Searches for new physics in precision atomic experiments

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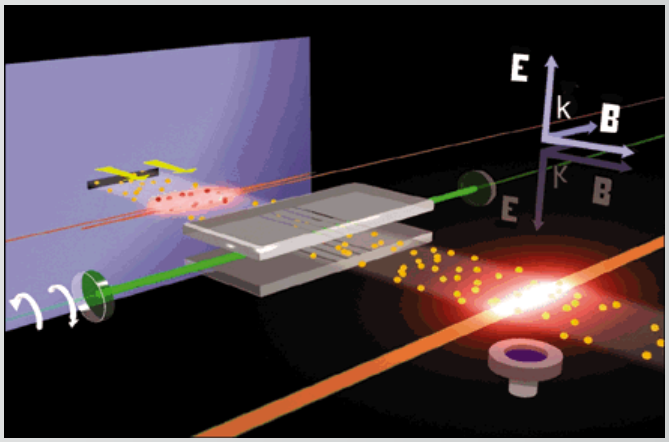
Australian Government
Australian Research Council



Canberra International Physics Summer School 2023 “Fields and Particles”

Plan

Lecture 1. How can atoms be used to test the SM and search for new physics?

- Atomic parity violation

Lecture 2. Time-reversal violating electric dipole moments

- Atomic EDMs, enhancement mechanisms

Lecture 3. Precision atomic theory

- Many-body methods, relativistic Hartree-Fock, QED in many-electron atoms

Lecture 4. Adventures at the intersection of atomic and nuclear physics

- Case study in the hyperfine structure

Lecture 3.
Precision atomic theory

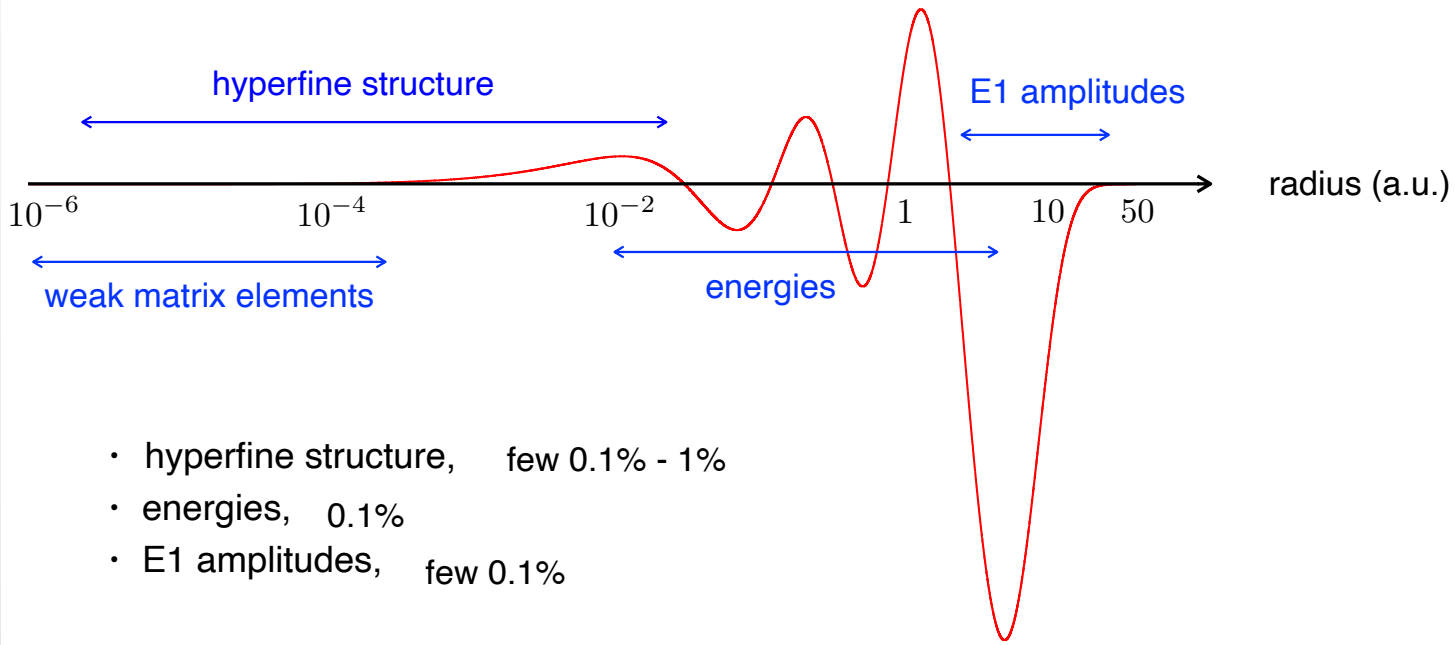
Our precision atomic theory group at UQ — goal

To maximise the discovery potential of precision atomic experiments

- Push state-of-the-art atomic calculations to 0.1% precision
  - Development of high-precision many-body methods
  - Improved benchmarking of atomic theory

Aim — accurate wave functions across all scales

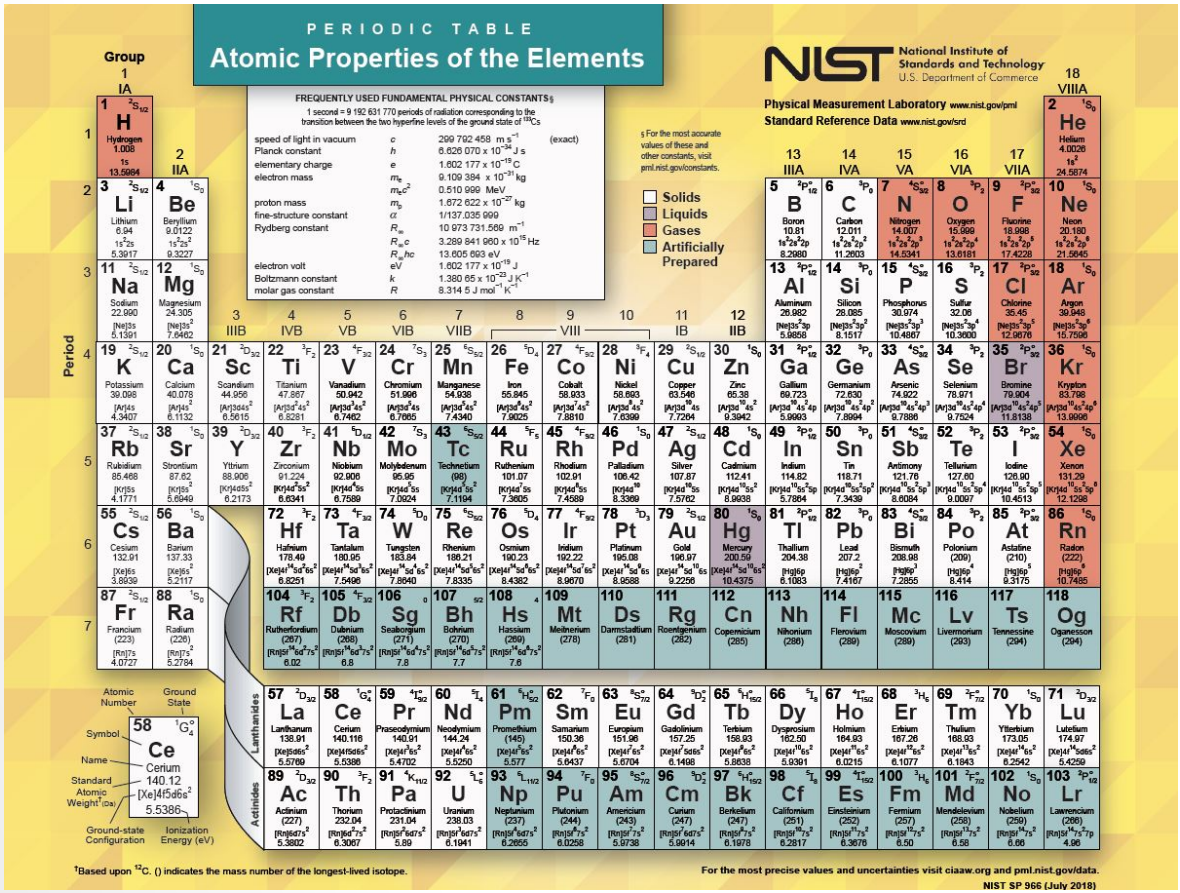
Upper radial component, Cs 6s:



- hyperfine structure, few 0.1% - 1%
- energies, 0.1%
- E1 amplitudes, few 0.1%

$$E_{\rm PV} = \sum_n \frac{\langle 7S_{1/2}|D|nP_{1/2}\rangle\langle nP_{1/2}|H_{\rm PV}|6S_{1/2}\rangle}{E_{6S_{1/2}} - E_{nP_{1/2}}} + \sum_n \frac{\langle 7S_{1/2}|H_{\rm PV}|nP_{1/2}\rangle\langle nP_{1/2}|D|6S_{1/2}\rangle}{E_{7S_{1/2}} - E_{nP_{1/2}}} = \xi Q_W$$

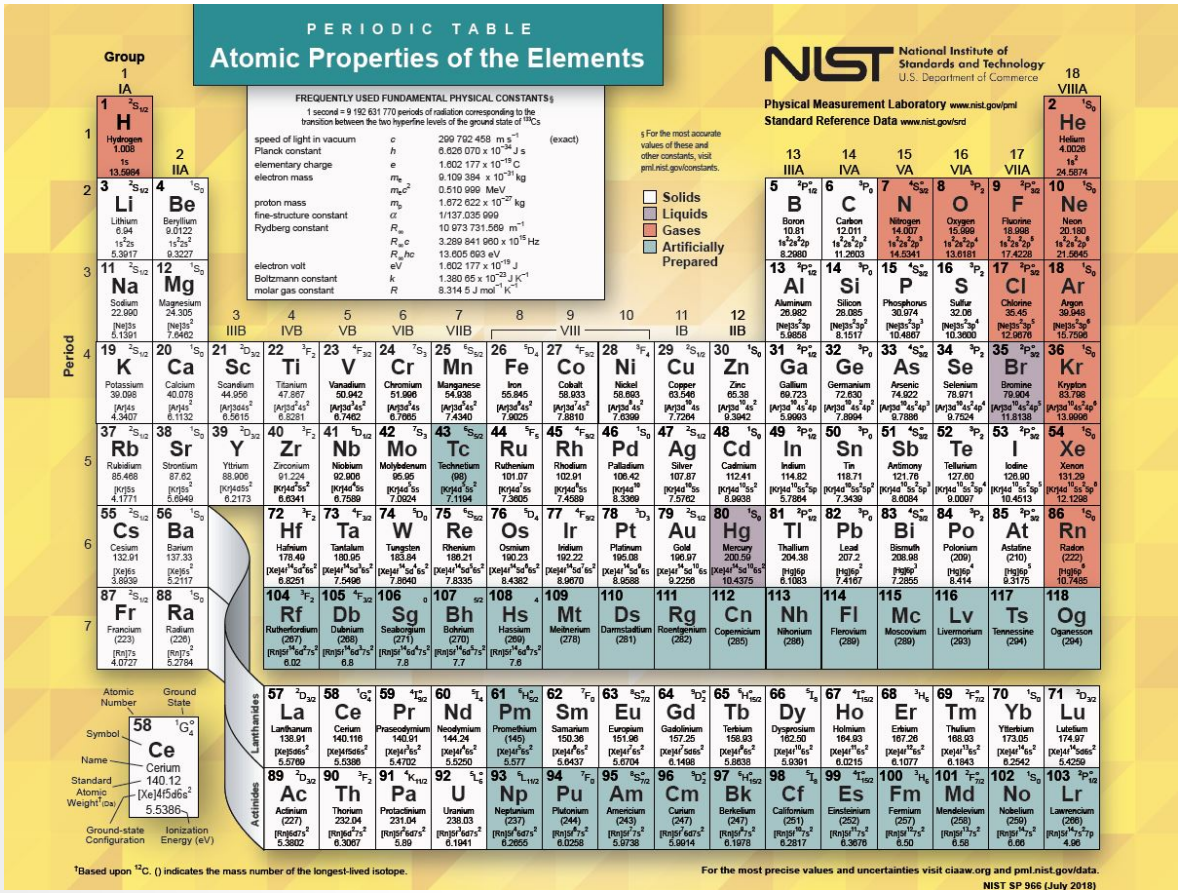
relativity



- Relativistic vs. non-relativistic

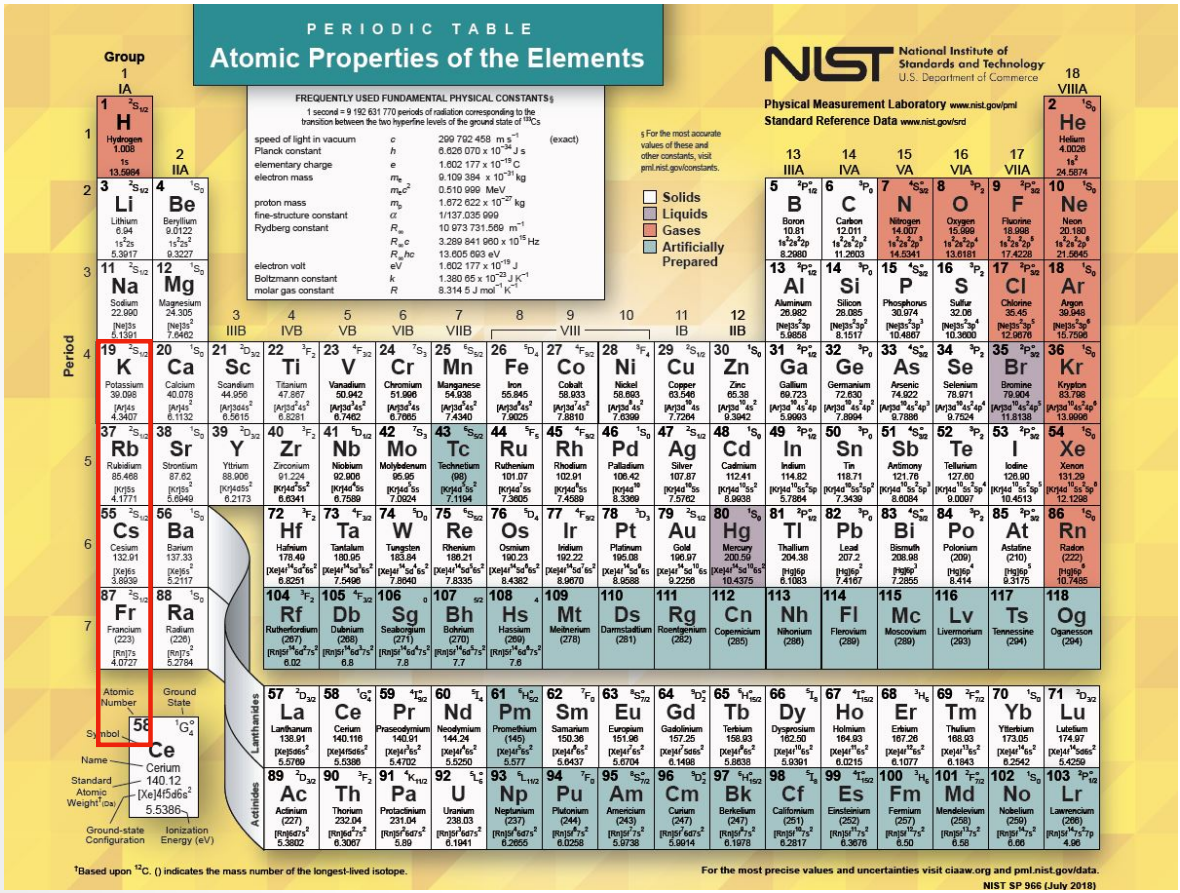
- How to treat correlations?

  Depends on how many valence electrons



number of valence electrons

- We will consider the theory for these atoms and ions



Overview

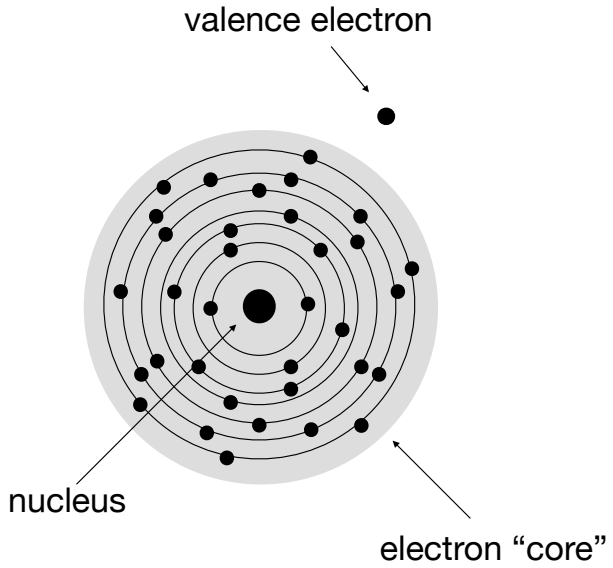
- Starting point for the many-electron problem: *relativistic Hartree-Fock (RHF)*

$$V_{\rm nuc} \to V_{\rm nuc} + V_{\rm HF}$$

- Beyond RHF: *the correlation potential*

$$V_{\rm HF} \to V_{\rm HF} + \Sigma$$

- QED radiative corrections: *vacuum polarisation and self-energy*



$$V_{\rm nuc} \to V_{\rm nuc} + V_{\rm rad}\,, \quad \text{radiative potential} \quad V_{\rm rad} = V_{\rm SE} + V_{\rm VP}$$

One-electron problem

Seek solution to: $h\varphi = \epsilon\varphi$

- Schrödinger Hamiltonian

$$h = \frac{p^2}{2m} + V(r) \ , \qquad V(r) = V_{\rm nuc}(r) + V_{\rm el}(r)$$

- Dirac Hamiltonian

$$h = c\boldsymbol{\alpha}\cdot\mathbf{p} + (\beta - 1)c^2 + V(r)$$

Dirac matrices: $\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix}, \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

Solution has form: $\varphi_{\kappa m}(\mathbf{r}) = \frac{1}{r}\begin{pmatrix} f_\kappa(r)\Omega_{\kappa m}(\mathbf{n}) \\ i\alpha g_\kappa(r)\Omega_{-\kappa m}(\mathbf{n}) \end{pmatrix}$

One-electron problem

Coupled radial equations:

$$-\left(\frac{d}{dr}+\frac{\kappa}{r}\right)f_\kappa+[\alpha^2(V_{\rm nuc}(r)+V_{\rm el})-2]g_\kappa=\alpha^2\epsilon g_\kappa$$

$$(V_{\rm nuc}(r)+V_{\rm el})f_\kappa+\left(\frac{d}{dr}-\frac{\kappa}{r}\right)g_\kappa=\epsilon f_\kappa$$

Express this as: $\dfrac{dy}{dr}=F(y,r)$

with $y=\begin{pmatrix} f_\kappa \\ g_\kappa \end{pmatrix}$

Solve using finite-difference method — Adams-Moulton

Method described in detail in: W. R. Johnson, *Atomic Structure Theory* (Springer, Berlin, 2007)

Solving the radial Dirac equation

In practice, we use a variable radial grid, point-spacing exponentially increasing at small distances, becoming linear at large distances

- start with solutions at large distances that satisfy the equation with potential

$$V(r) = (N - Z - 1)/r$$

  and integrate inwards

- Integrate outwards starting with solutions at small distances where

$$V(r) \approx -Z/r$$

- Meet at outer turning point

Method described in detail in: W. R. Johnson, *Atomic Structure Theory* (Springer, Berlin, 2007)

Solving the radial Dirac equation

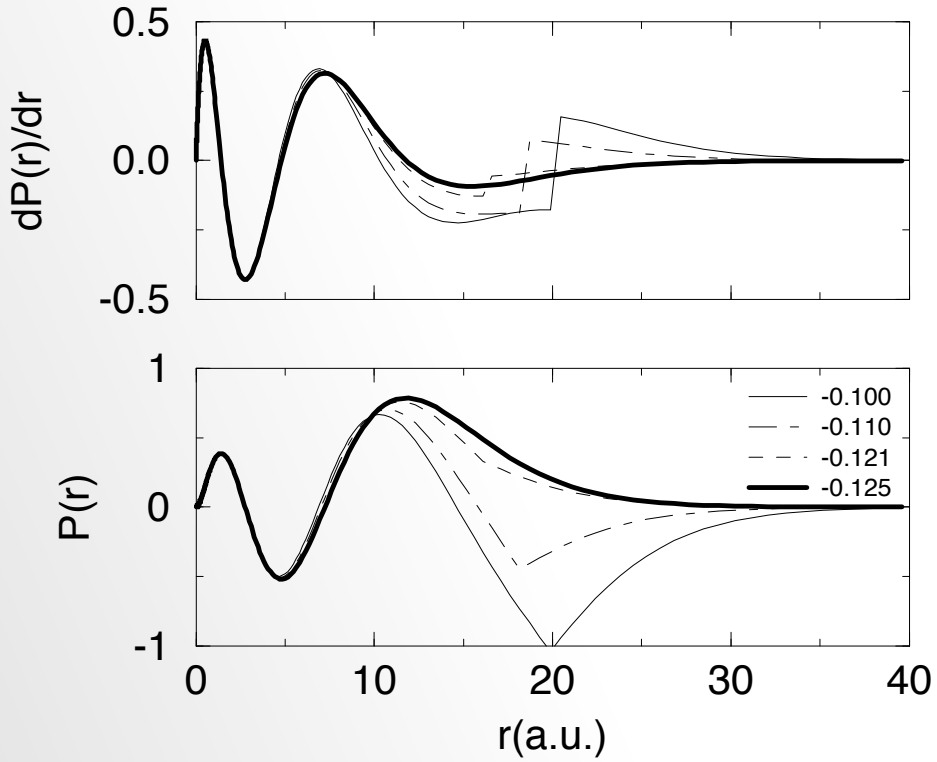


Illustration of matching:
radial 4p orbital
(non-relativistic)
in Coulomb potential

Check number of “zeros”

$$n = n_0 + l + 1$$

Crude adjustment to
energy until correct

Fine adjustment until
function and derivative
are smooth

Method described in detail in: W. R. Johnson, *Atomic Structure Theory* (Springer, Berlin, 2007)

Relativistic Hartree-Fock

- Hamiltonian for many-electron atom:

$$H = \sum_{i=1}^{N} h_0(\mathbf{r}_i) + \sum_{i<j}^{N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$

- Wish to solve

$$H\Phi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = E\Phi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)$$

It is perhaps worthwhile repeating here an observation by Hartree (1957, p. 16) concerning "exact" solutions to Eq.(3.38) in the many-electron case. If we consider, for example, the 26 electron iron atom, the function $\Psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$ depends on $3 \times 26 = 78$ variables. Using a course grid of only 10 points for each variable, it would require 10^{78} numbers to tabulate the wave function for iron. Since this number exceeds the estimated number of particles in the solar system, it is difficult to understand how the wave function would be stored even if it could be calculated! Of more practical interest are approximations to "exact" solutions and methods for systematically improving the accuracy of such approximations.

From: W. R. Johnson, *Atomic Structure Theory* (Springer, Berlin, 2007)

Relativistic Hartree-Fock

- Hamiltonian for many-electron atom:

$$H = \sum_{i=1}^{N} h_0(\mathbf{r}_i) + \sum_{i<j}^{N} \frac{1}{|\mathbf{r}_i - \mathbf{r}_j|}$$

- Wish to solve

$$H\Phi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) = E\Phi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N)$$

- Approximate solution — single Slater determinant

$$\Phi(\mathbf{r}_1, \mathbf{r}_2, ..., \mathbf{r}_N) \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_a(\mathbf{r}_1) & \varphi_b(\mathbf{r}_1) & \cdots & \varphi_n(\mathbf{r}_1) \\ \varphi_a(\mathbf{r}_2) & \varphi_b(\mathbf{r}_2) & \cdots & \varphi_n(\mathbf{r}_2) \\ \vdots & & & \\ \varphi_a(\mathbf{r}_N) & \varphi_b(\mathbf{r}_N) & \cdots & \varphi_n(\mathbf{r}_N) \end{vmatrix}$$

where $h\varphi_a = (h_o + U(r))\varphi_a = \epsilon_a \varphi_a$

Relativistic Hartree-Fock

- Expectation value of full Hamiltonian: $E = \langle \Phi | H | \Phi \rangle$
- Require that the energy is stationary with respect to variations of the radial wave functions, subject to the normalisation condition
- Finally, obtain relativistic Hartree-Fock equations, with potential:

$$V_{HF} R_a(r) = \sum_b (2j_b + 1) \Big[\underbrace{v_0(b,b,r) R_a(r)}_{\text{direct}} - \underbrace{\sum_k \Lambda_{\kappa_a k \kappa_b} v_k(b,a,r) R_b(r)}_{\text{exchange}} \Big] \ .$$

where

$$\begin{aligned} v_k(a,b,r) &= \int_0^\infty dr' \frac{r_<^k}{r_>^{k+1}} \Big[f_a(r') f_b(r') + \alpha^2 g_a(r') g_b(r') \Big] \ , \\ \Lambda_{\kappa_a k \kappa_b} &= \begin{pmatrix} j_a & j_b & k \\ -1/2 & 1/2 & 0 \end{pmatrix}^2 \Pi(l_a + k + l_b) \ , \end{aligned}$$

$$\Pi(l) = \begin{cases} 1 \ , & l \text{ even} \\ 0 \ , & l \text{ odd} \end{cases} \ .$$

Relativistic Hartree-Fock

- Solving the RHF equations, $V_{\rm el} = V_{HF}$

$$-\left(\frac{d}{dr} + \frac{\kappa}{r}\right) f_\kappa + [\alpha^2 (V_{\rm nuc}(r) + V_{\rm el}) - 2] g_\kappa = \alpha^2 \epsilon g_\kappa$$

$$(V_{\rm nuc}(r) + V_{\rm el}) f_\kappa + \left(\frac{d}{dr} - \frac{\kappa}{r}\right) g_\kappa = \epsilon f_\kappa$$

- Self-consistently for electrons of core
- Freeze potential of core, V_{HF}^{N-1}
- Solve for valence electron in V_{HF}^{N-1}

Correlation potential

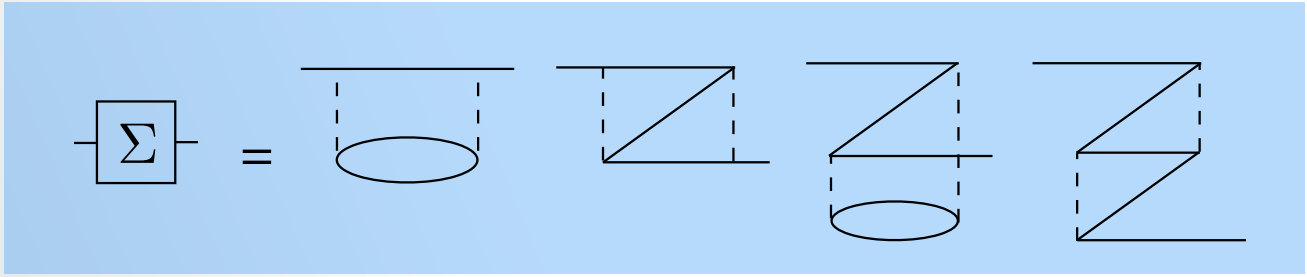
- Starting point: relativistic Hartree-Fock (RHF),

$$\left[c\boldsymbol{\alpha}\cdot\mathbf{p}+(\beta-1)c^2-Z/r+V_{\rm HF}\right]\varphi=\epsilon\varphi$$

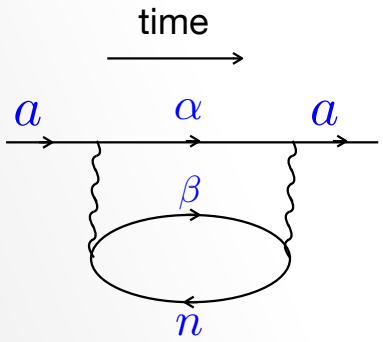
Excitation energies, error ~ 10%

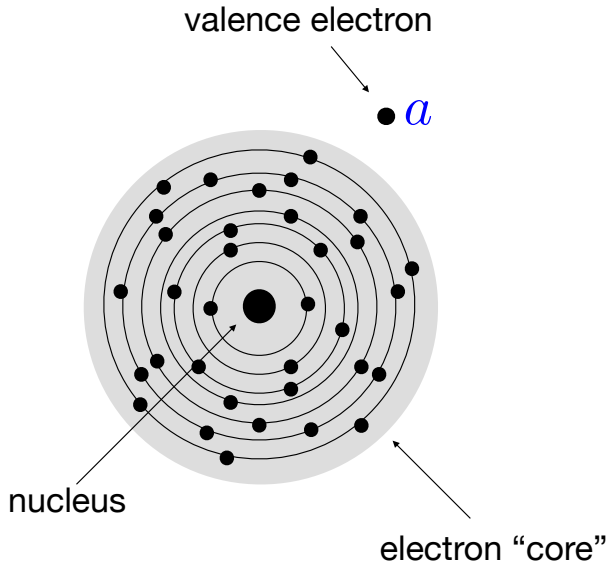
- Perturbation theory in residual Coulomb interaction, $\sum_{i<j}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}-\sum_i V_{{\rm HF},i}$

- Lowest-order correlation corrections - 2nd order in Coulomb interaction



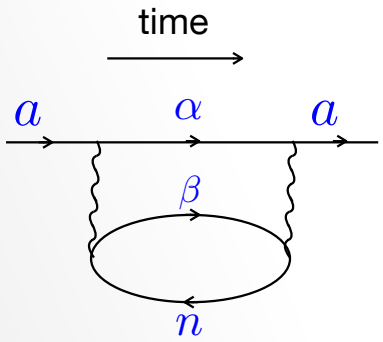
Correlation potential

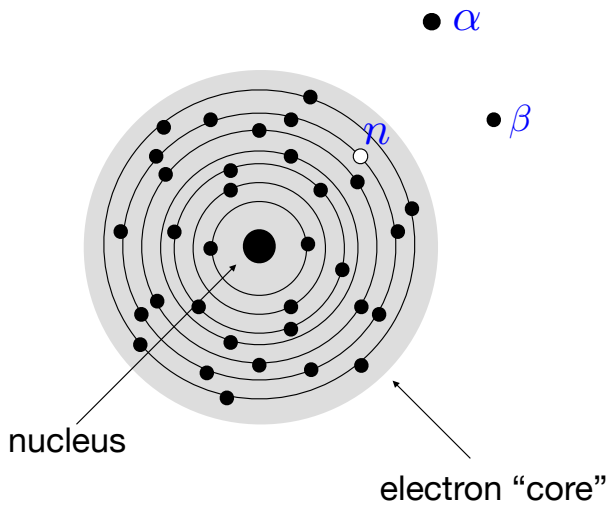




$$\langle a|\Sigma|a\rangle = \sum_{n,\alpha,\beta} \frac{\langle an|\frac{1}{r_{24}}|\beta\alpha\rangle\langle\beta\alpha|\frac{1}{r_{13}}|na\rangle}{\epsilon_a + \epsilon_n - \epsilon_\alpha - \epsilon_\beta}$$

Correlation potential





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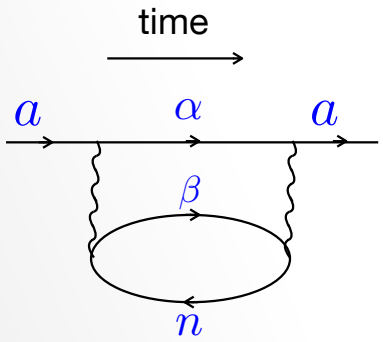
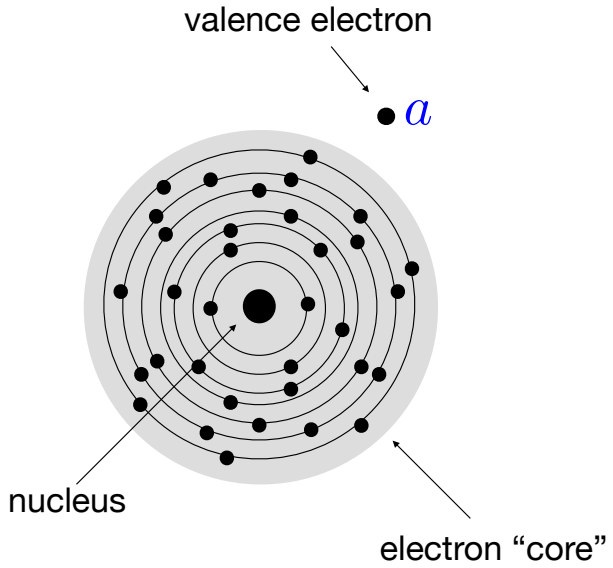
Correlation potential





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Correlation potential

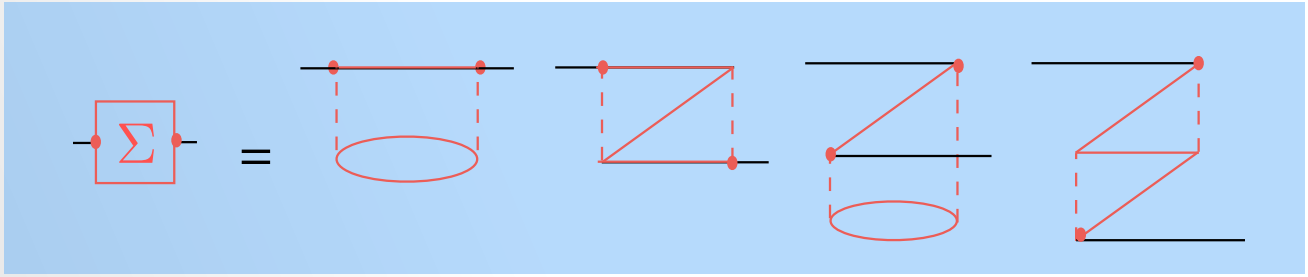
- Starting point: relativistic Hartree-Fock (RHF),

$$\left[c\boldsymbol{\alpha}\cdot\mathbf{p}+(\beta-1)c^2-Z/r+V_{\rm HF}\right]\varphi=\epsilon\varphi$$

Excitation energies, error ~ 10%

- Perturbation theory in residual Coulomb interaction, $\sum_{i<j}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}-\sum_i V_{{\rm HF},i}$

- Lowest-order correlation corrections - 2nd order in Coulomb interaction



- Pull out the *correlation potential* and add it to the Hartree-Fock equations,

$$V_{HF}\Rightarrow V_{HF}+\Sigma(\mathbf{r},\mathbf{r}',\epsilon)$$

Correlation potential

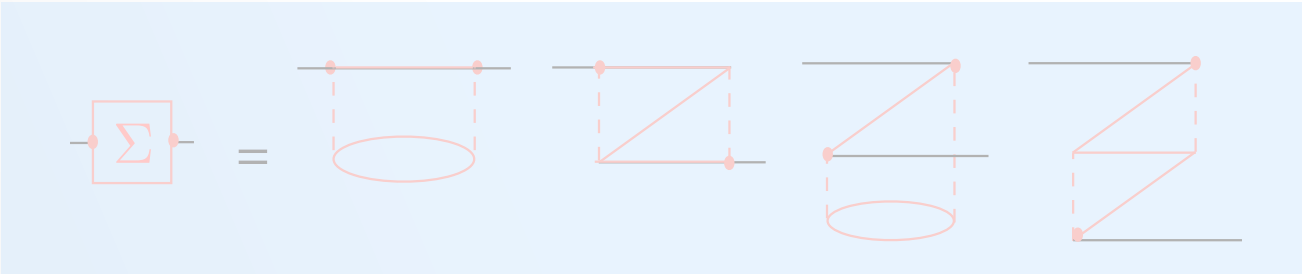
- Starting point: relativistic Hartree-Fock (RHF),

$$\left[c\boldsymbol{\alpha}\cdot\mathbf{p}+(\beta-1)c^2-Z/r+V_{\rm HF}+\Sigma\right]\varphi_{\rm Br}=\epsilon_{\rm Br}\varphi_{\rm Br}$$

Excitation energies, error ~ 1%

- Perturbation theory in residual Coulomb interaction, $\sum_{i<j}\frac{1}{|\mathbf{r}_i-\mathbf{r}_j|}-\sum_i V_{{\rm HF},i}$

- Lowest-order correlation corrections - 2nd order in Coulomb interaction

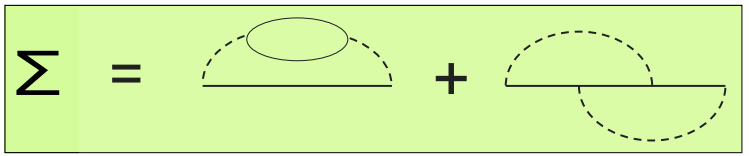


- Pull out the *correlation potential* and add it to the Hartree-Fock equations,

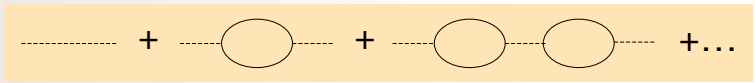
$$V_{HF}\Rightarrow V_{HF}+\Sigma(\mathbf{r},\mathbf{r}',\epsilon)$$

All-orders correlation potential

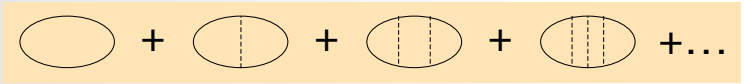
Classes of diagrams included to all orders using the Feynman diagram technique



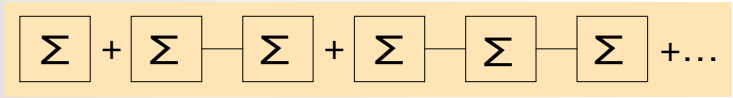
1. Electron-electron screening

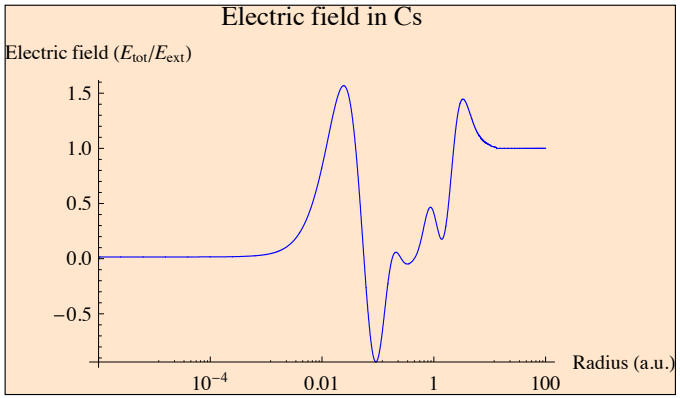


2. Hole-particle interaction



Non-linear-in- Σ contributions

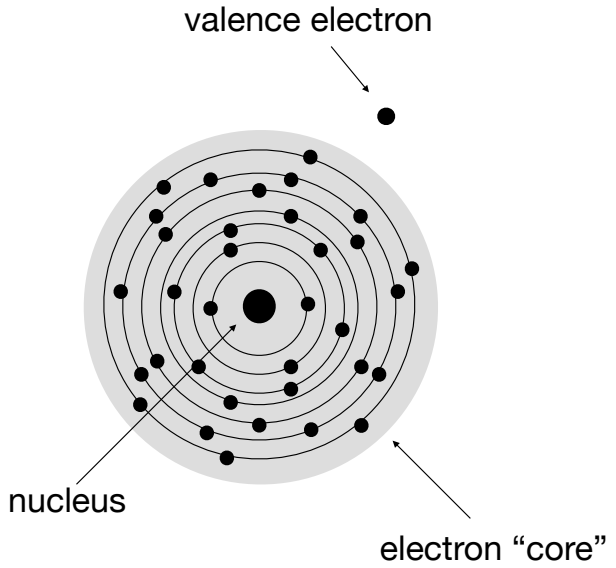




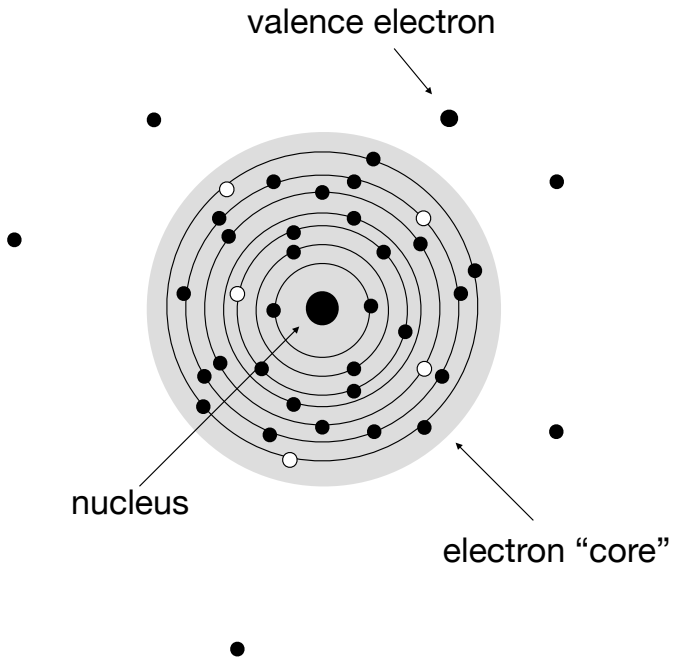
Excitation energies, error ~ 0.1%

Dzuba, Flambaum, Sushkov (1989)

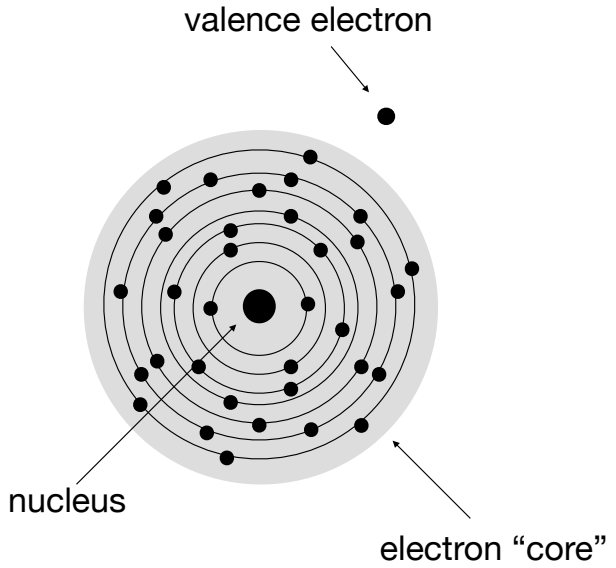
All-orders correlation potential



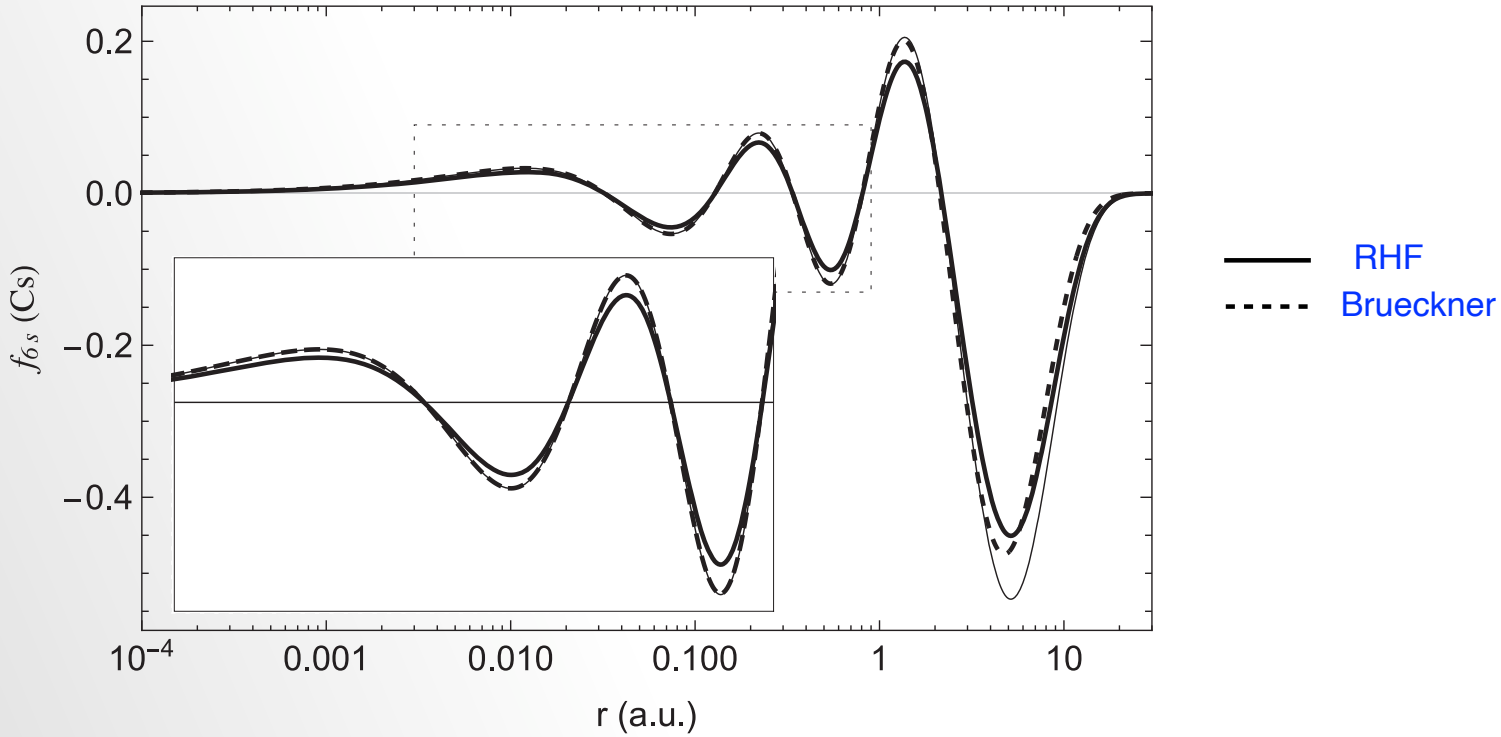
All-orders correlation potential



All-orders correlation potential

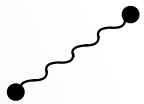


Affect on wave function



“Small corrections”

Breit corrections

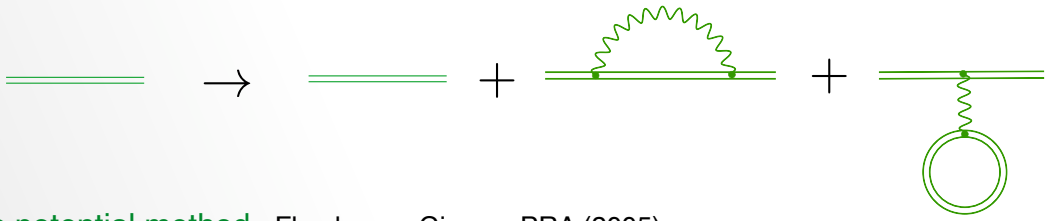


Retardation and magnetic corrections to Coulomb interaction

$$\frac{1}{r} \;\to\; \frac{1}{r} - \frac{1}{2r}\Big(\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j + \boldsymbol{\alpha}_i \cdot \mathbf{n}\; \boldsymbol{\alpha}_j \cdot \mathbf{n}\Big)$$

where $\mathbf{r} = \mathbf{n}r = \mathbf{r}_i - \mathbf{r}_j$

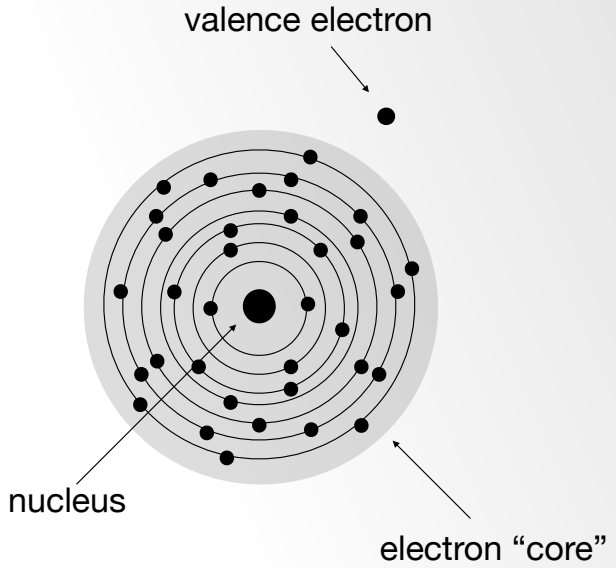
QED corrections in many-body calculations



Radiative potential method - Flambaum, Ginges, PRA (2005)

Model operator approach - Shabaev, Tupitsyn, Yerokhin, PRA (2013)

“Small corrections”



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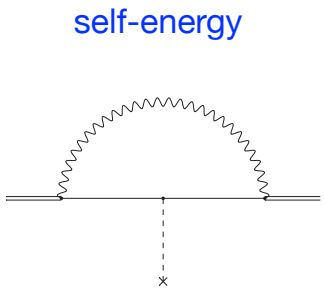

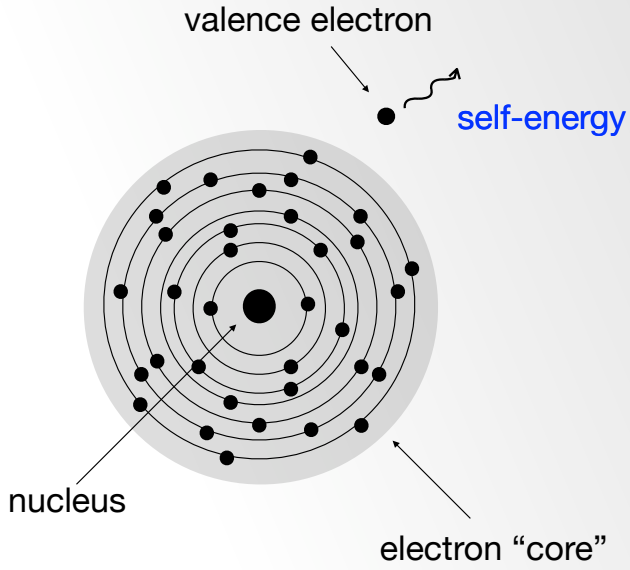

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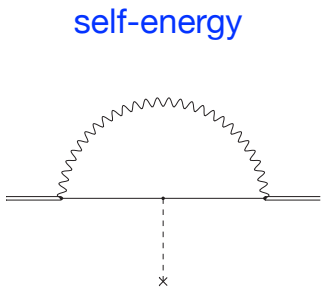
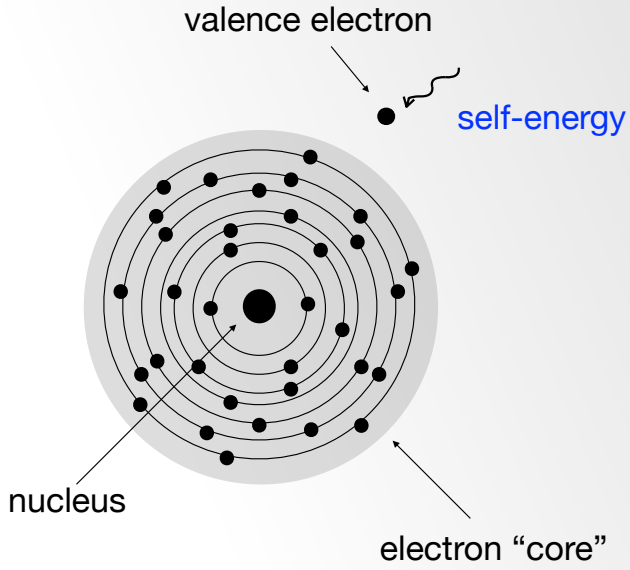
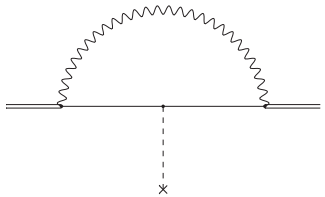


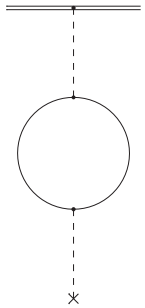


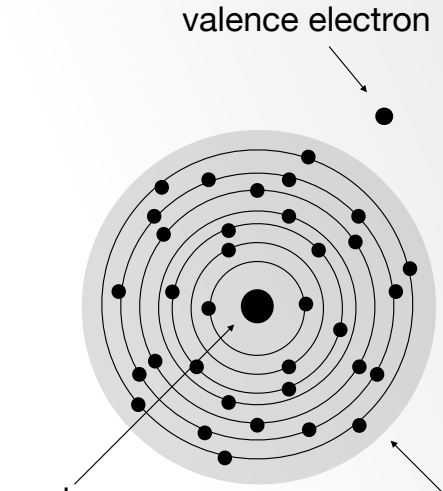
“Small corrections”

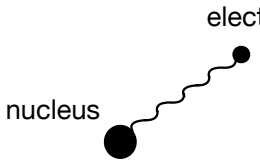
self-energy



vacuum polarisation







vacuum polarisation

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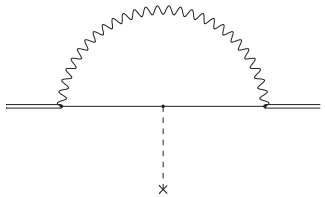
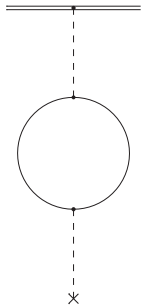
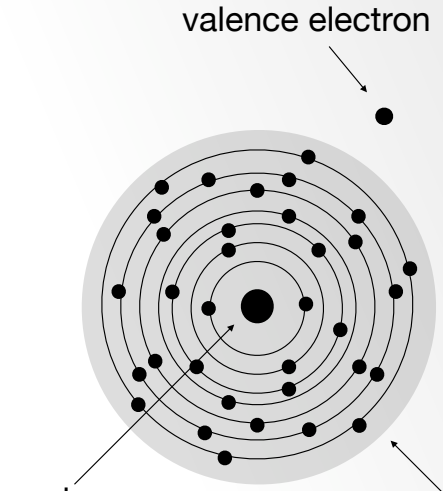
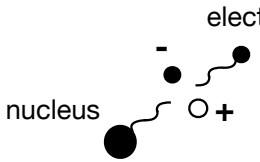


vacuum polarisation







vacuum polarisation

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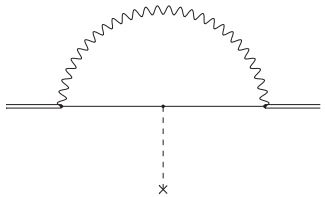
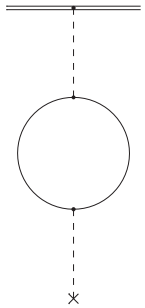
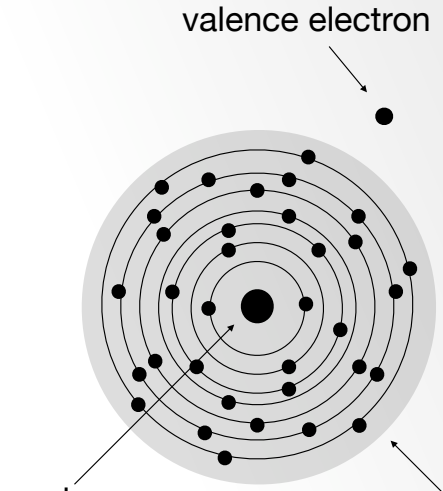
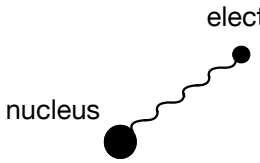
self-energy



vacuum polarisation







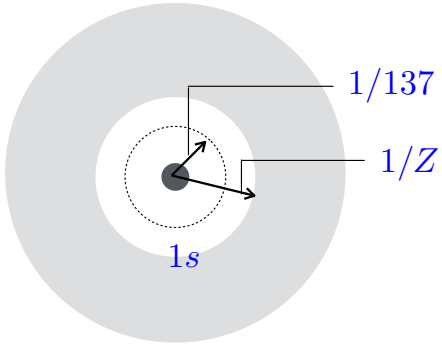
vacuum polarisation

Radiative potential

Typical range of quantum electrodynamics radiative interactions

$$r \sim \hbar/mc \approx 1/137 \,\text{a.u.}$$

within the 1s orbit, $r \sim 1/Z$

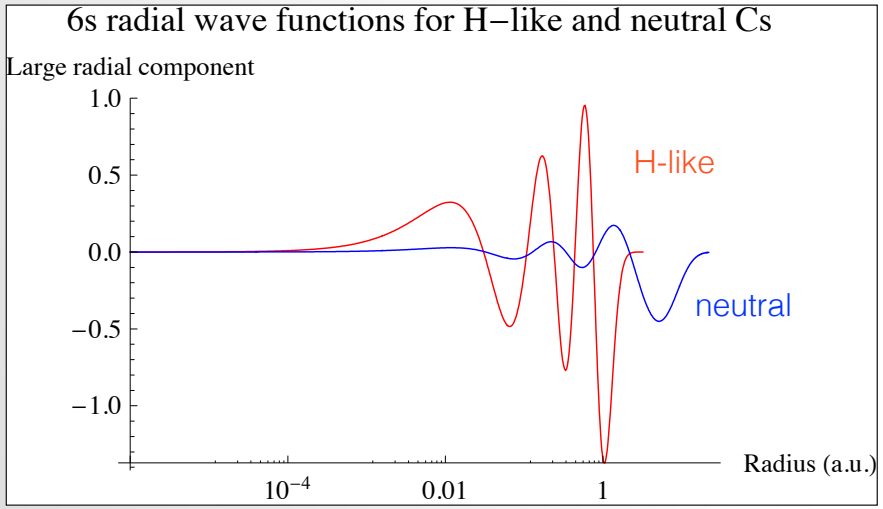


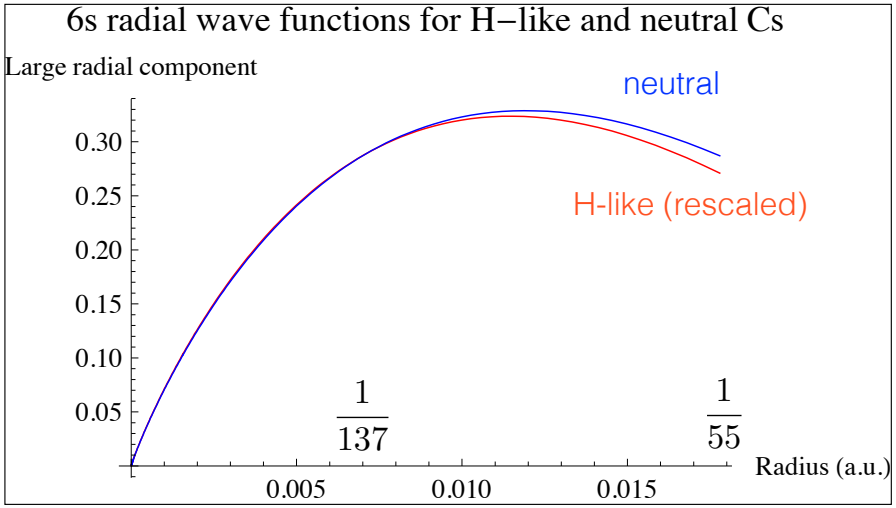
Electron sees unscreened nucleus, $V \approx -Z/r$

Binding energies of valence electrons, $\epsilon \sim 10^{-5} mc^2$

In this region, valence electron of a neutral atom behaves like an electron in a highly-excited state of a hydrogen-like ion!

Radiative potential





Radiative potential

- Define radiative potential: $\langle\varphi|V_{\rm rad}(r)|\varphi\rangle = \delta\epsilon_{SE} + \delta\epsilon_{VP}$

Note: $$\frac{\langle\varphi|V_{\rm rad}|\varphi\rangle}{\rho(r_n)} = \frac{\langle\varphi|V_{\rm rad}|\varphi\rangle_{\rm H-like}}{\rho(r_n)_{\rm H-like}}$$

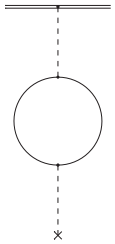
- Introduce local radiative potential:

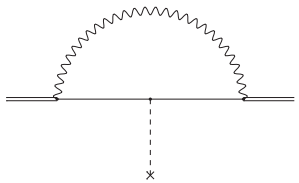
$$V_{\rm rad}(r) = V_{\rm Ueh}(r) + V_{\rm mag}(r) + V_{\rm el}^{\rm high}(r) + V_{\rm el}^{\rm low}(r)$$

First order in $Z\alpha$ vacuum polarization — Uehling potential

Ab initio derivation to first order in $Z\alpha$; cut-off imposed for electric part

Approximation to long-range electric part. Semi-empirical





Flambaum, Ginges (2005)

Radiative potential

- Define radiative potential: $\langle\varphi|V_{\rm rad}(r)|\varphi\rangle = \delta\epsilon_{SE} + \delta\epsilon_{VP}$

Note: $$\frac{\langle\varphi|V_{\rm rad}|\varphi\rangle}{\rho(r_n)} = \frac{\langle\varphi|V_{\rm rad}|\varphi\rangle_{\rm H-like}}{\rho(r_n)_{\rm H-like}}$$

- Introduce local radiative potential:

$$V_{\rm rad}(r) = V_{\rm Ueh}(r) + V_{\rm mag}(r) + V_{\rm el}^{\rm high}(r) + V_{\rm el}^{\rm low}(r)$$

- Fitting factors found by reproducing SE shifts in exact QED to H-like ions

$$V_{\rm mag}^{\rm point}(\mathbf{r}) = -\frac{i\alpha^2}{4\pi}\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}\left[\left(\frac{Z}{r}\right)\left(\int_1^\infty dt\,\frac{1}{t^2\sqrt{t^2-1}}e^{-2tr/\alpha} - 1\right)\right],$$

$$V_{\rm high}^{\rm point}(r) = A_l(Z,r)\left(\frac{\alpha}{\pi}\right)\left(\frac{Z}{r}\right)\int_1^\infty dt\,\frac{1}{\sqrt{t^2-1}}\left[\left(1-\frac{1}{2t^2}\right)[\ln(t^2-1)+4\ln(1/Z\alpha+1/2)] - \frac{3}{2} + \frac{1}{t^2}\right]e^{-2tr/\alpha},$$

$$V_{\rm low}^{\rm point}(r) = B_l(Z)Z^4\alpha^3 e^{-Zr}$$

Flambaum, Ginges (2005)

Radiative potential

Self-energy shifts and comparison to exact QED

In frozen atomic potential (Kohn-Sham)

$$\delta\epsilon_{\rm SE} = \frac{\alpha}{\pi}\frac{(Z\alpha)^4}{n^3}F(Z\alpha)mc^2$$

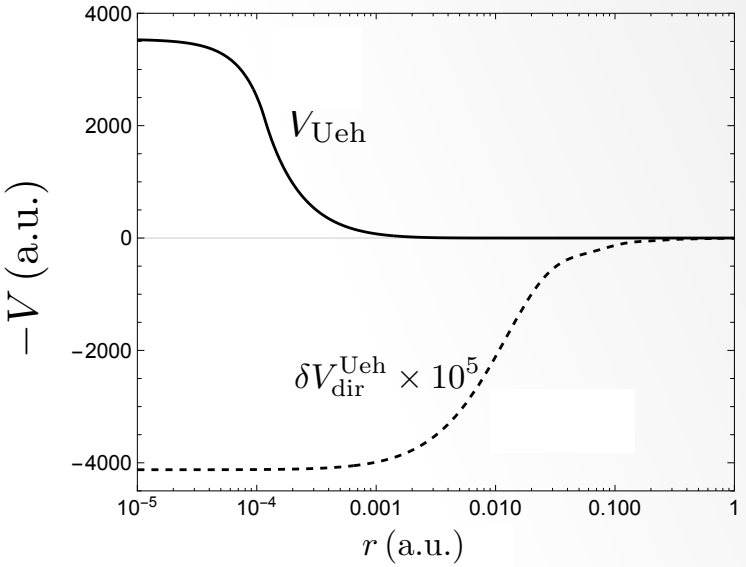
$F(Z\alpha)$

		Radiative potential	Radiative potential + screening	Exact QED	Model Operator
Cs	6s	0.0167	0.0164	0.0162	0.0163
Fr	7s	0.0099	0.0098	0.0098	0.0099

Core relaxation is important!

SE shifts for Cs. Units: 10^{-5} a.u.

	$\delta\epsilon^{(1)}$	$+\delta\epsilon^{\rm relax}$
$6s_{1/2}$	8.13	8.43
$6p_{1/2}$	0.11	-0.38
$6p_{3/2}$	0.32	-0.09
$5d_{3/2}$	-0.06	-1.21
$5d_{5/2}$	0.07	- 1.12



Uehling potential and induced (direct) Hartree-Fock potential for Cs

What else?

- This is a *snapshot* of some of our methods
- Need to go further to:
  - take into account external fields
  - consider multi-valence electron atoms
- There are other high-precision methods out there

Summary

Lecture 3. Precision atomic theory

- Many-body methods, relativistic Hartree-Fock, QED in many-electron atoms

Next. Adventures at the intersection of atomic and nuclear physics

- Case study in the hyperfine structure