Numerical Implementation of the Relativistically Covariant Many-Body Perturbation Theory

A status report from the Gothenburg group

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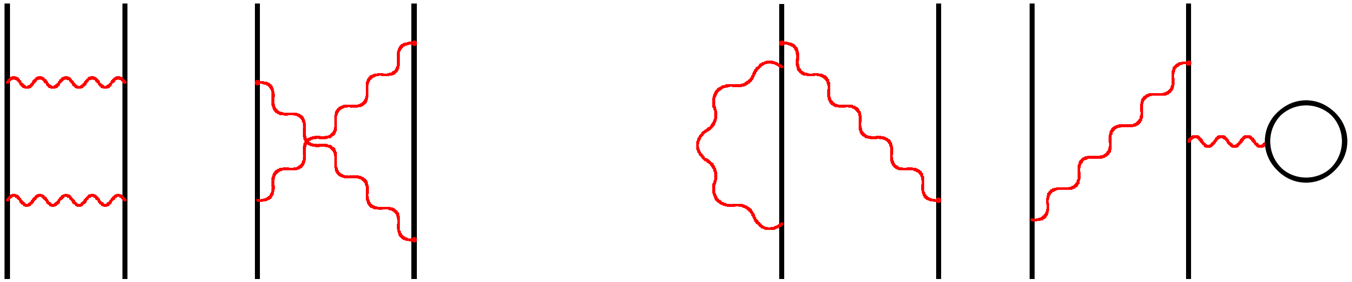
Calculations of He-like systems

- The $Z\alpha$-expansion
  - H. Araki & J. Sucher
  - G.W.F. Drake, K. Pachucki & J. Sapirstein
- Many-Body Perturbation Theory, MBPT
  - Relativistic MBPT, (D.R. Plante *et al.*& I. Lindgren *et al.*)
- Numerical Basis Set - QED calculations
  - S-matrix formalism
  - Covariant-Evolution-Operator Method, (I. Lindgren *et al.*)
  - The Two-Times Greens Function Method, (V.M. Shabaev *et al.*)

Numerical Basis Set - QED calc.

- The Two-Photon Effects



Photon Exchange　　　　Radiative Effects

- B. Åsén *et al.*, Phys. Rev. A 65, 032516 (2002)
- A.N. Artemyev *et al.*, Phys. Rev. A 71, 062104 (2005)

Numerical Basis Set - QED calc.

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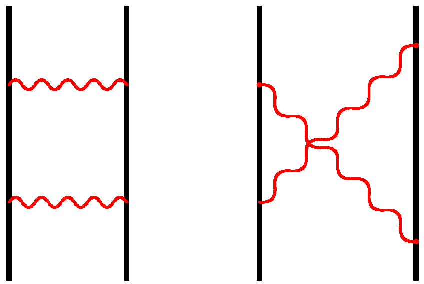
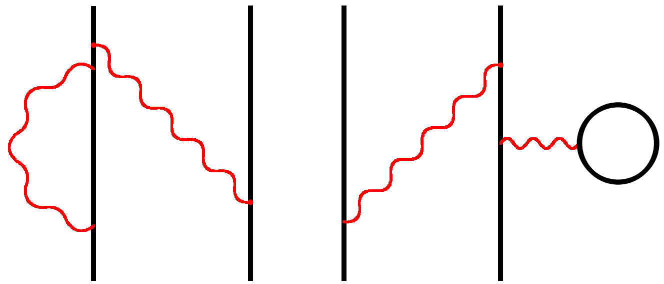


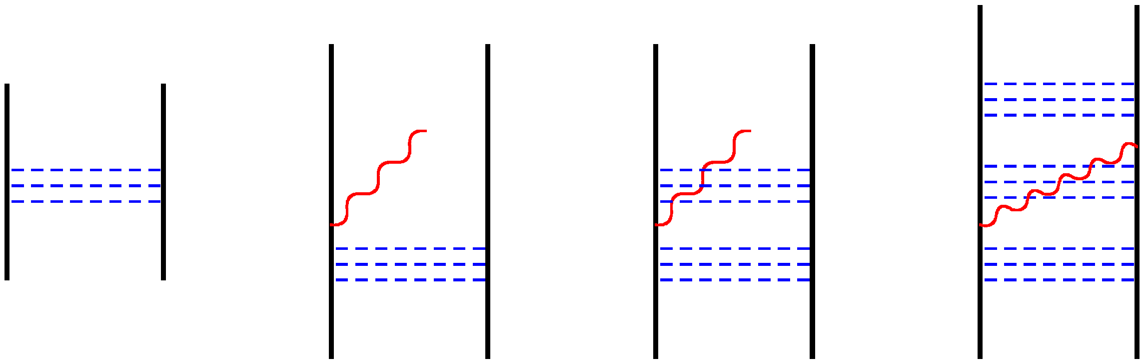
Photon Exchange



Radiative Effects

  - B. Åsén *et al.*, Phys. Rev. A 65, 032516 (2002)
  - A.N. Artemyev *et al.*, Phys. Rev. A 71, 062104 (2005)

- QED Calculations with Correlated Numerical WaveFunctions



Heavy-Ion Research

- The FAIR project - The new experimental facilities under construction at GSI-Darmstadt, Germany
  - FLAIR - Facility for Low-Energy Antiproton and Ions Research
  - SPARC - Stored Particle Atomic physics Research Collaboration

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"At present, this interplay between QED and many-body effects constitutes the greatest challenge posed to the accurate theoretical evaluation of transition energies in the field of highly charged heavy ions".

S. Fritzsche, T. Stölker & P. Indelicato, J. Phys. B: At. Mol. Opt. Phys **38** (2005)

Helium Fine Structure, 1s2p

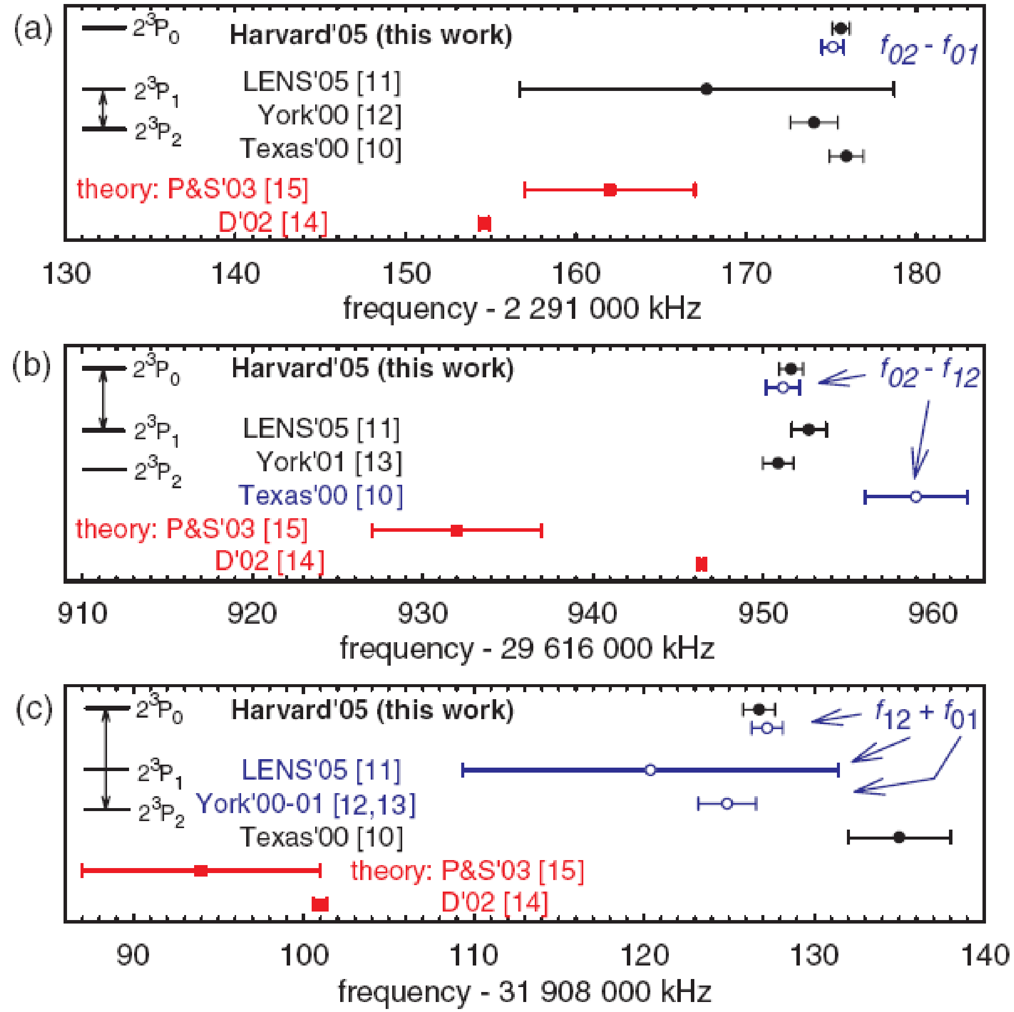
Independent determination of the fine-structure constant α

Experimental values,

- G. Gabrielse *et al.*, Harvard
- E.A. Hessels *et al.*, York
- M. Inguscio *et al.*, LENS
- J. Castillega *et al.*, Texas

Theoretical results,

- G.W.F. Drake
- K. Pachucki & J. Sapirstein



T. Zelevinsky *et al.*, PRL 95 (2005)

Outline

- Short Presentation of the Theories
  - Many-Body Perturbation Theory
  - Covariant-Evolution-Operator Method
- Theoretical and Numerical Results
  - No virtual pair calculations
  - Virtual Pairs
- Future Prospects

Many-Body Perturbation Theory

- Time-independent perturbation theory, $H = H_0 + V$.
- The wave operator transforms the unperturbed states into their exact target states, $|\Psi^\alpha\rangle = \Omega|\Phi^\alpha\rangle$.
- The energy is given by the effective Hamiltonian, H_{eff}.
  - $H_{\text{eff}}|\Phi^\alpha\rangle = E^\alpha|\Phi^\alpha\rangle$
  - $H_{\text{eff}} = PH\Omega P = PH_0P + PV\Omega P$
- Degeneracy & Quasi-Degenracy
  - Extended Model Space
  - $P + Q = \mathbf{1}$
- Generalized Bloch equation

$$[\Omega, H_0]P = V\Omega P - \Omega P V \Omega P$$

Std Relativistic MBPT

- Dirac-Coulomb Approximation

$$H = \mathbf{\Lambda}_+ \Big[\sum_{i=1}^{N} h_D(i) + \sum_{i<j}^{N} \frac{e^2}{4\pi r_{ij}} \Big] \mathbf{\Lambda}_+$$

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- Dirac-Coulomb-Breit Approximation

$$H = \mathbf{\Lambda}_+ \Big[\sum_{i=1}^{N} h_D(i) + \sum_{i<j}^{N} \frac{e^2}{4\pi r_{ij}} + H_B \Big] \mathbf{\Lambda}_+$$

$$H_B = -\frac{e^2}{8\pi} \sum_{i<j} \Big[\frac{\alpha_i \cdot \alpha_j}{r_{ij}} + \frac{(\alpha_i \cdot r_{ij})(\alpha_j \cdot r_{ij})}{r_{ij}^3} \Big]$$

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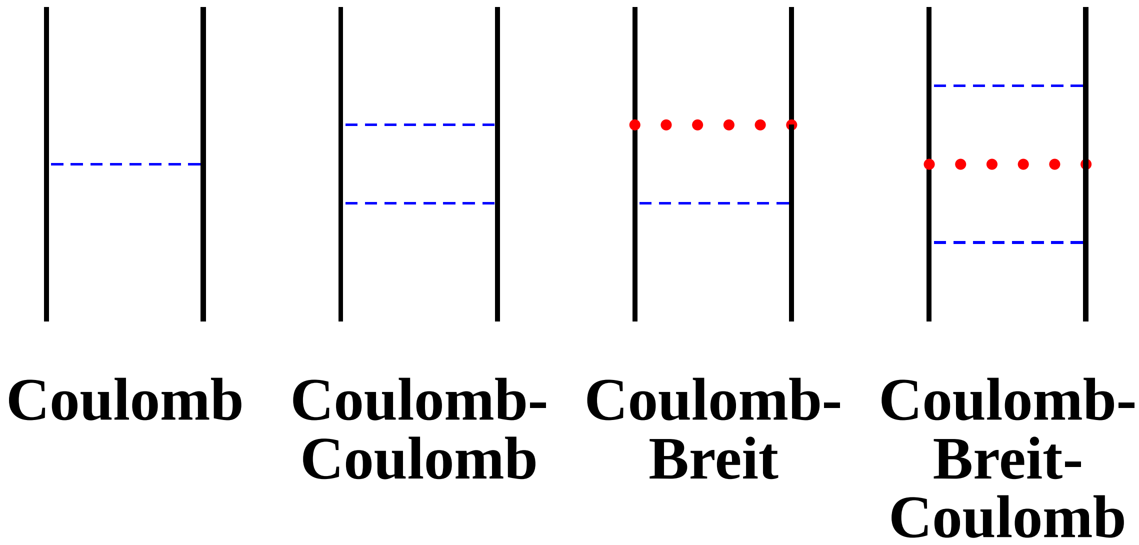
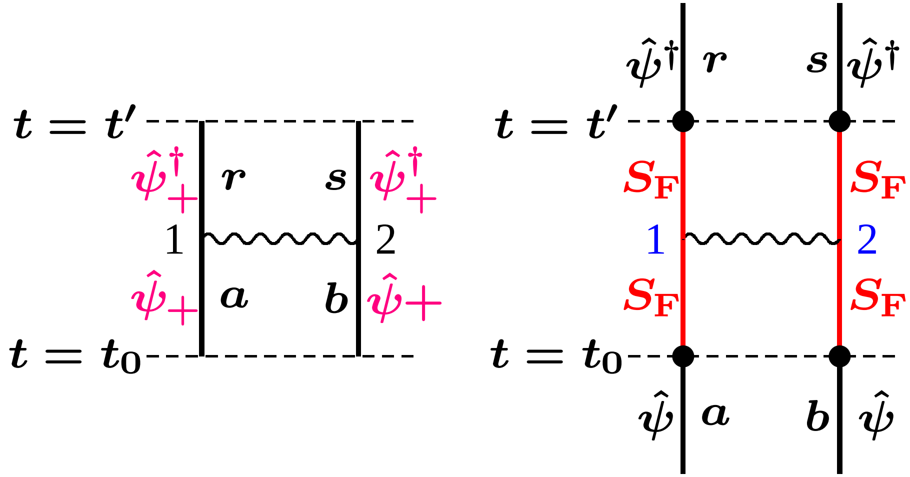
  - **No QED effects**
  - **Not Relativistically Covariant**
  - **Correct to order** α^2

Diagrammatic Representation of

Dirac-Coulomb-Breit Approximation for Helium-like Systems



Covariant Evolution Operator



- Original time evolution operator is non-covariant
  - No outgoing or incoming electron states with negative energy
- Insertion of zeroth-order Green's function

$$U^{(2)}_{\rm Cov}(t',-\infty) = -\frac{1}{2}\iint d^3x'_1 d^3x'_2\ \hat{\psi}^\dagger(x'_1)\hat{\psi}^\dagger(x'_2)$$

$$\times\iint d^4x_1 d^4x_2\ G_0(x'_1,x'_2;x_1,x_2)\iint d^3x'_{10}d^3x'_{20}\ {\rm i}I(x_1,x_2)$$

$$\times G_0(x_1,x_2;x_10,x_20)\hat{\psi}(x_{10})\hat{\psi}(x_{20})\,{\rm e}^{-\gamma(|t_1|+|t_2|)}$$

- Integration of t_1 and t_2 is performed over all time

C.E.O. Method

- Reduced time-evolution operator, $\widetilde{U}(t)$

$$\begin{aligned} \widetilde{U}(t) &= U'_{\text{Cov}}(t)P - \widetilde{U}(t)P \cdot PU'_{\text{Cov}}(0)P \\ U'_{\text{Cov}}(t) &= U_{\text{Cov}}(t) - 1 \end{aligned}$$

  - The (quasi)-singularities in $U'_{\text{Cov}}(t)P$ are cancelled by the corresponding terms in the counterterm $\widetilde{U}(t)P \cdot PU'_{\text{Cov}}(0)P$, which results in a regular reduced time-evolution operator.

- Wave operator for time-dependent interactions

$$\Omega = [1 + Q\widetilde{U}(0)]$$

- Review article about the C.E.O Method
  - Physics Reports 389, 161-261 (2004)

The TV chef trick

- Recipe
  - Phys. Rev. A 73, 062502 (2006)
  - Can. J. Phys. 83, 183-218 (2005)

Bloch Equations

- Generalized Bloch equation

$$[\Omega_{\mathrm{I}}, H_0]P = V_{12}\Omega_{\mathrm{I}}P - \Omega_{\mathrm{I}}P \cdot V_{\mathrm{eff}}$$

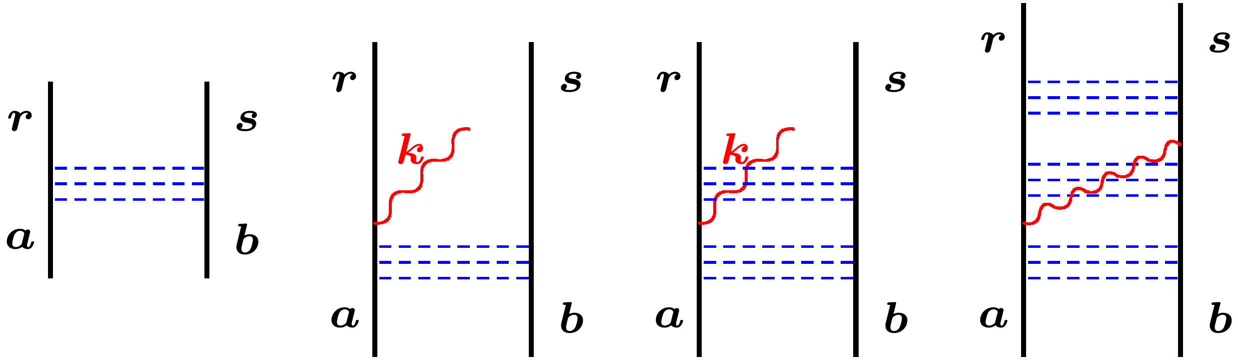
- Bloch equation with an "uncontracted" photon

$$[\Omega^l(k), H_0]P = V_k^l\Omega_{\mathrm{I}}P + V_{12}\Omega^l(k)P - \Omega^l(k)P \cdot V_{\mathrm{eff}}$$

- Bloch equation with a "contracted" photon

$$[\Omega_{\mathrm{ph}}, H_0]P = V_k^l\Omega^l(k) + V_{12}\Omega_{\mathrm{ph}}P - \Omega_{\mathrm{ph}}P \cdot V_{\mathrm{eff}}$$

Our Production Line, NVP



(a) (b) (c) (d)

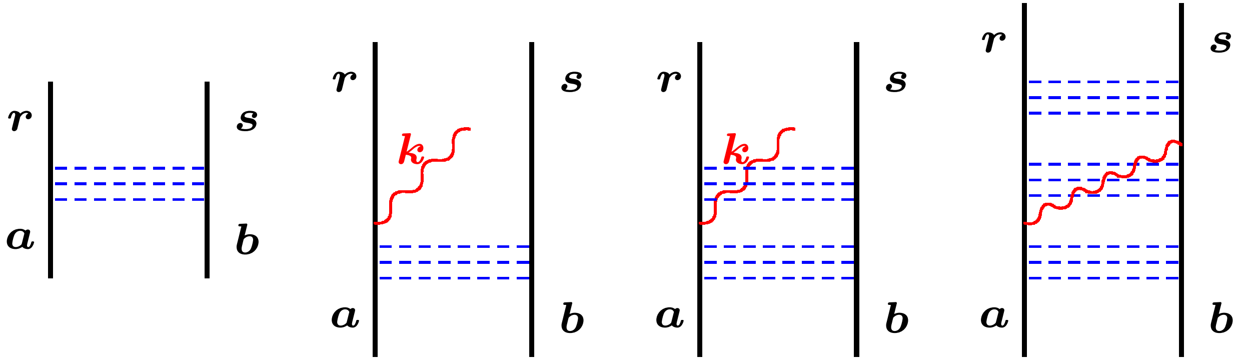
- Instantaneous Coulomb interactions, V_{12} (a)

$$\big(\mathcal{E}-H_0\big)|\rho_{ab}\rangle = |rs\rangle\langle rs|V_{12}|\rho_{ab}\rangle - |\rho_{cd}\rangle\langle cd|V_{\rm eff}|ab\rangle$$

- One retarded interaction (b)

$$\big(\mathcal{E}-H_0-k\big)|\rho^l_{ab}(k)\rangle = |rs\rangle\langle rs|V^l(k)|\rho_{ab}\rangle - |\rho^l_{cd}(k)\rangle\langle cd|V_{\rm eff}|ab\rangle$$

Our Production Line, NVP



(a) (b) (c) (d)

- Crossing Coulomb interactions (c)

$$\begin{aligned}\big(\mathcal{E}-H_0-k\big)|\rho^l_{ab}(k)\rangle &= |rs\rangle\langle rs|V^l(k)|\rho_{ab}\rangle \\ &+ |rs\rangle\langle rs|V_{12}|\rho^l_{ab}(k)\rangle - |\rho^l_{cd}(k)\rangle\langle cd|V_{\rm eff}|ab\rangle\end{aligned}$$

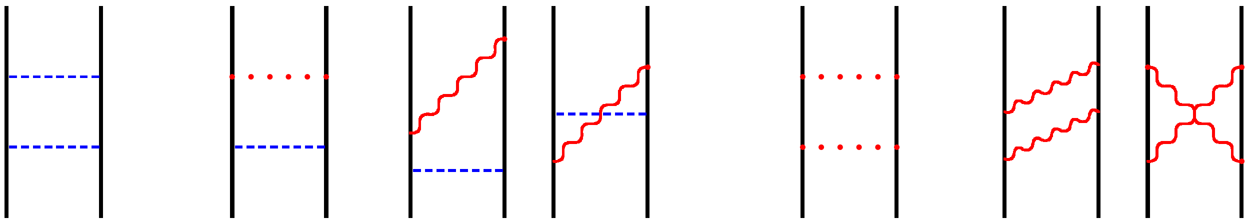
- Absorbing photon, additional Coulomb interactions (d)

$$\begin{aligned}\big(\mathcal{E}-H_0\big)|\rho_{{\rm ph},ab}\rangle &= |rs\rangle\langle rs|V^l(k)|\rho^l_{ab}(k)\rangle \\ &+ |rs\rangle\langle rs|V_{12}|\rho_{{\rm ph},ab}\rangle - |\rho_{{\rm ph},cd}\rangle\langle cd|V_{\rm eff}|ab\rangle\end{aligned}$$

Numerical results

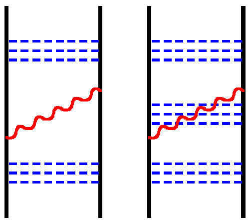
He-like neon ground state, non-rad. effect with No-Virtual Pairs (in μH)

Coul.-Coul. **Coulomb-Breit** (unretarded, retard.) **Breit-Breit** (unretarded, retard.)



NVP: -158 000 -2870 122 -46 13

+ Correlation



-57 15

Numerical results

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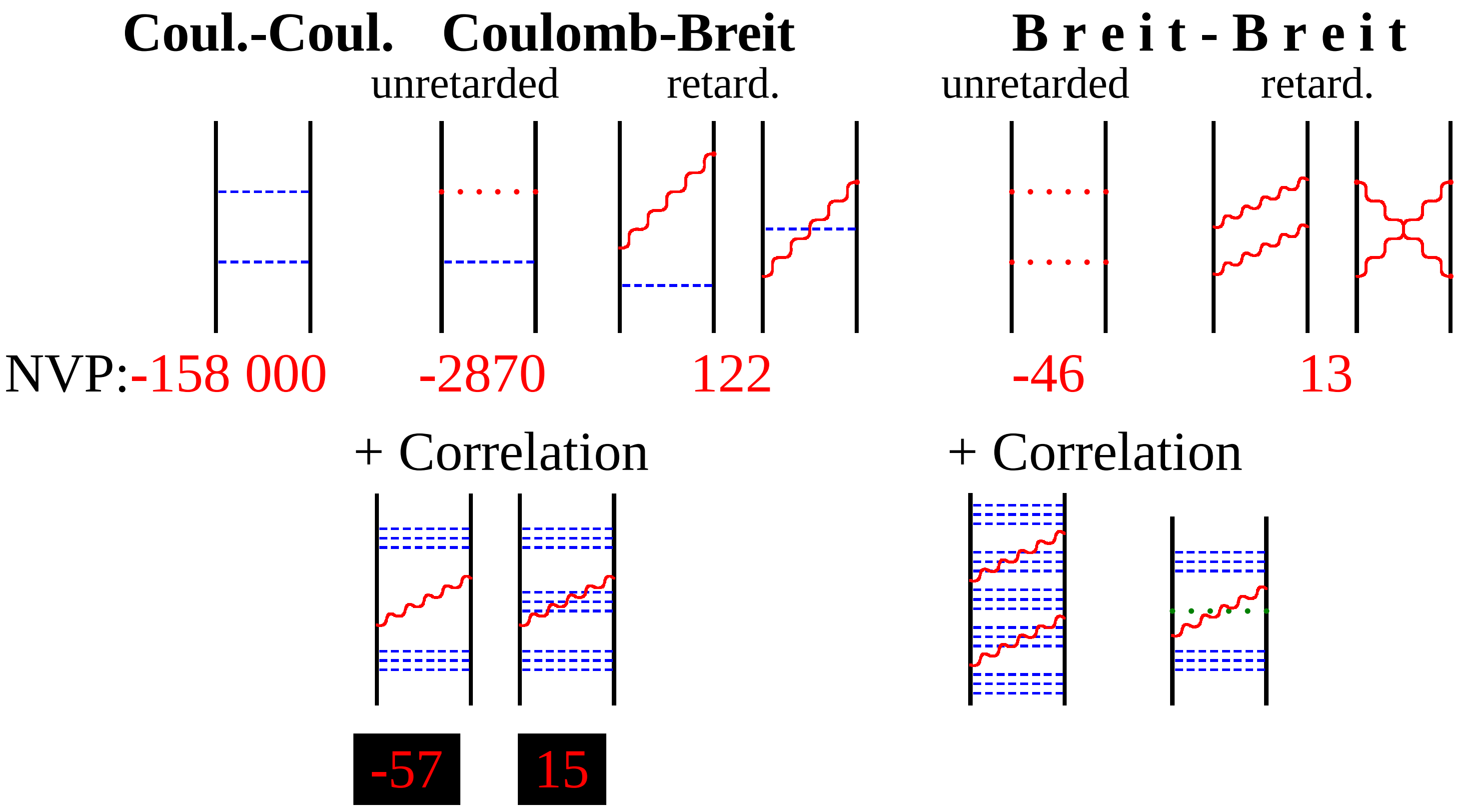
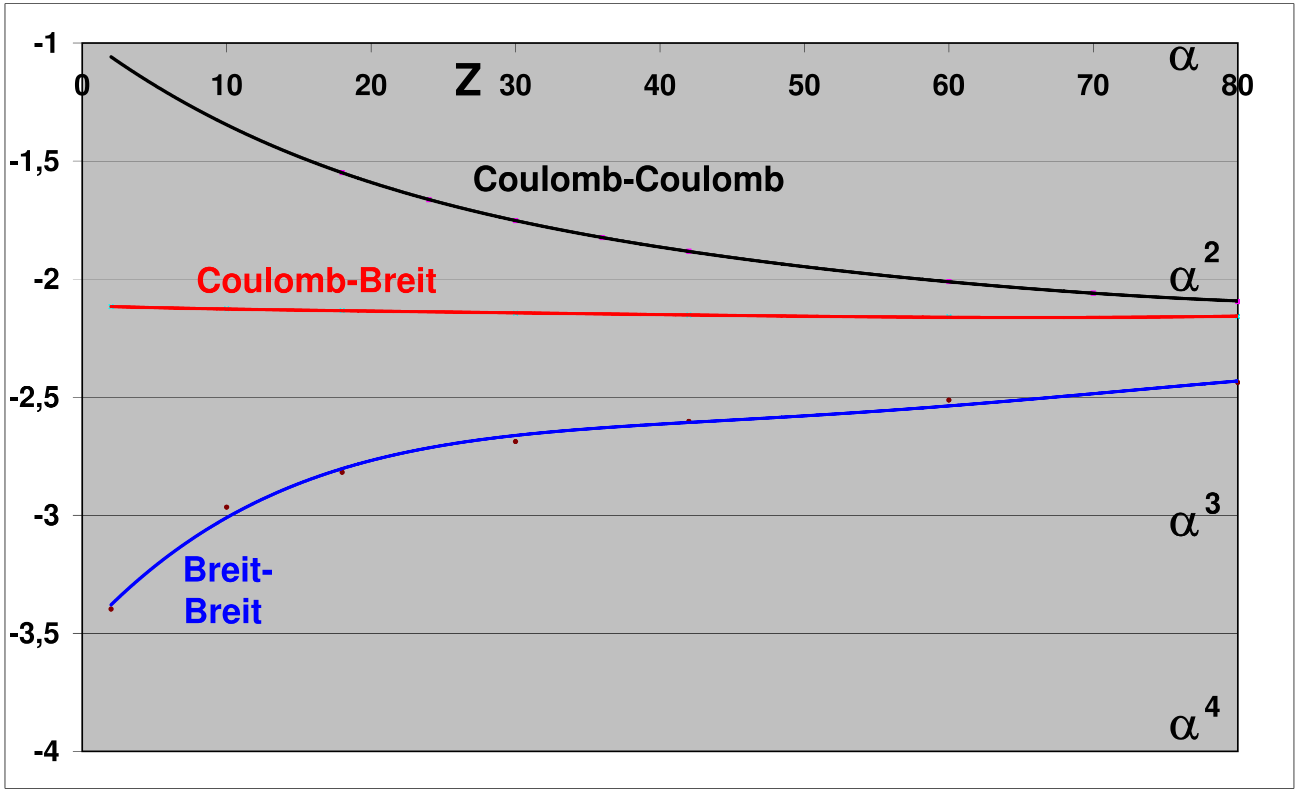
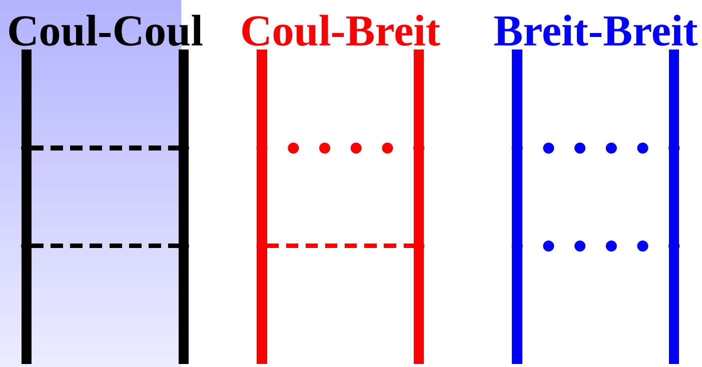


He-like Ions

Dirac-Coulomb-Breit

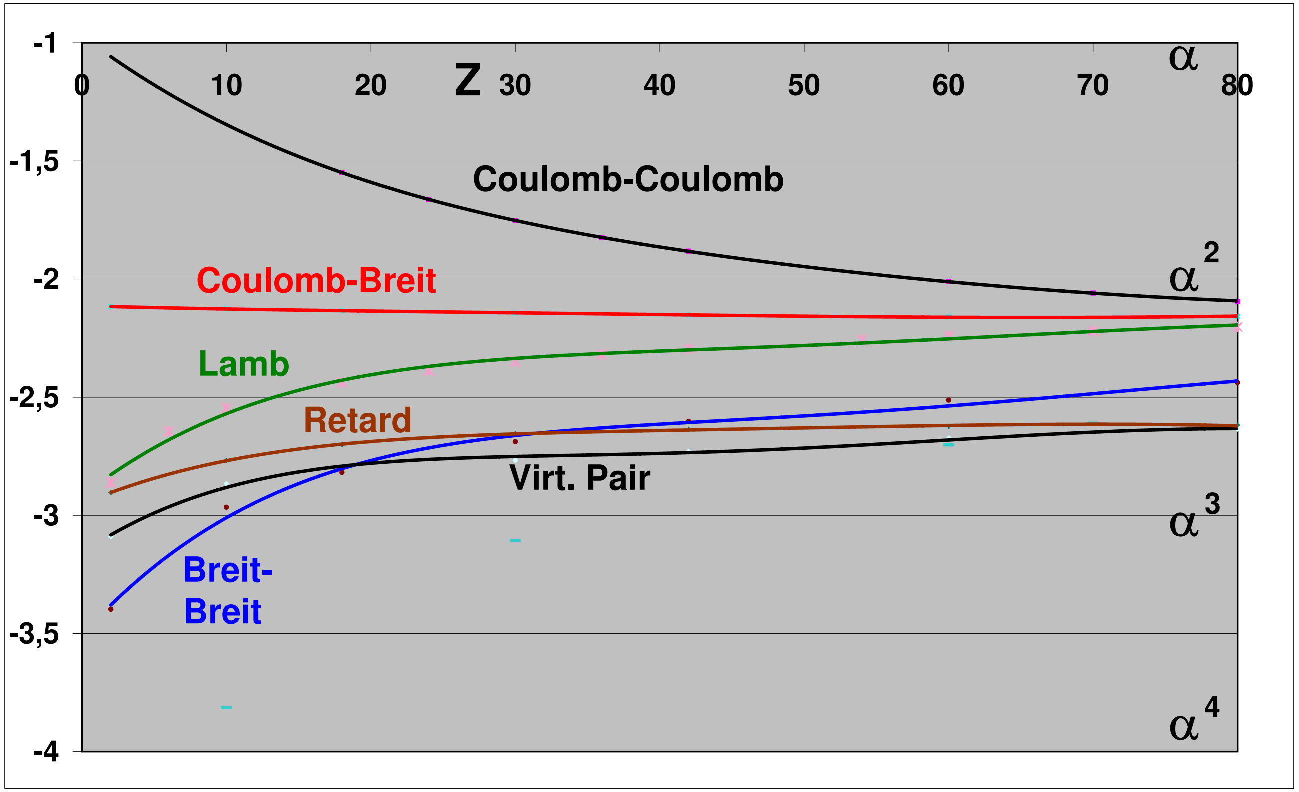


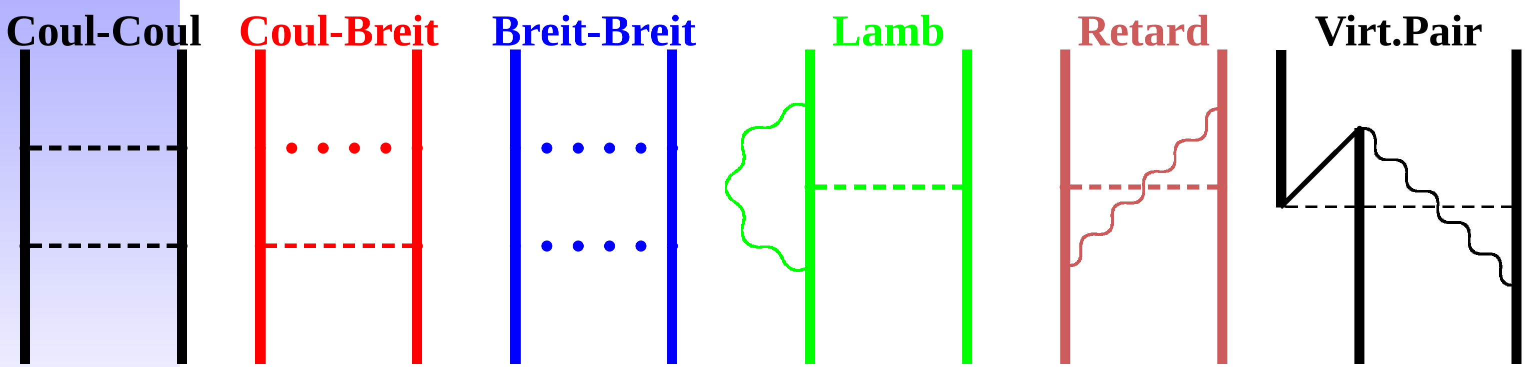


He-like Ions

Dirac-Coulomb-Breit

1st Order QED



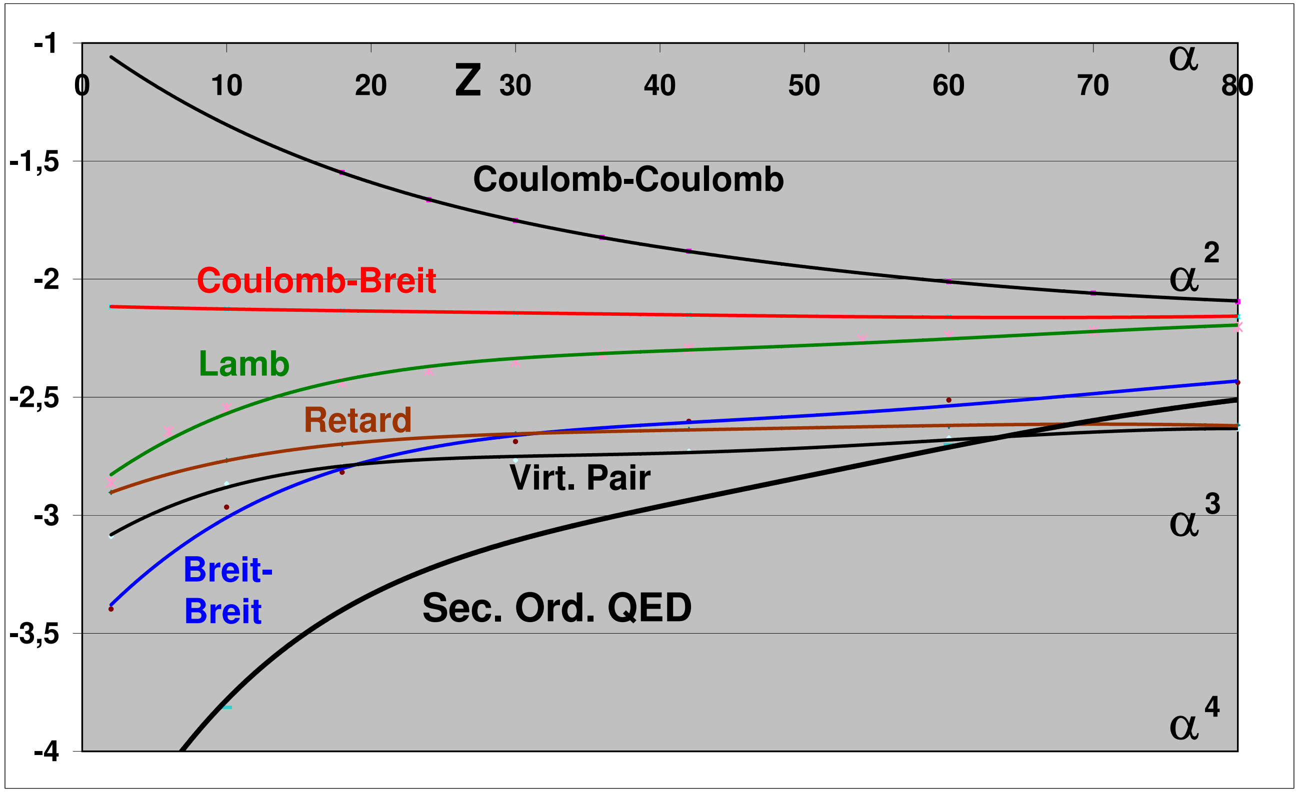


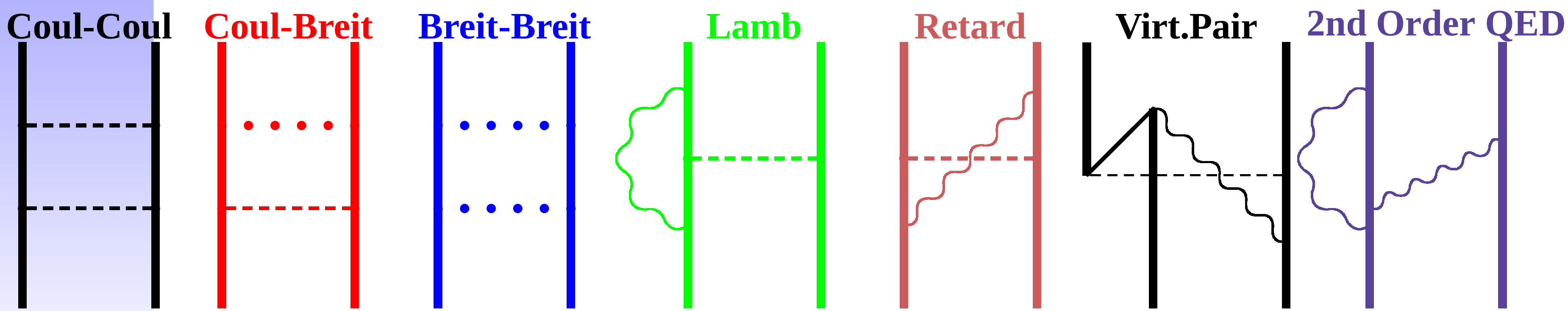
He-like Ions

Dirac-Coulomb-Breit

1st Order QED

2nd Order QED





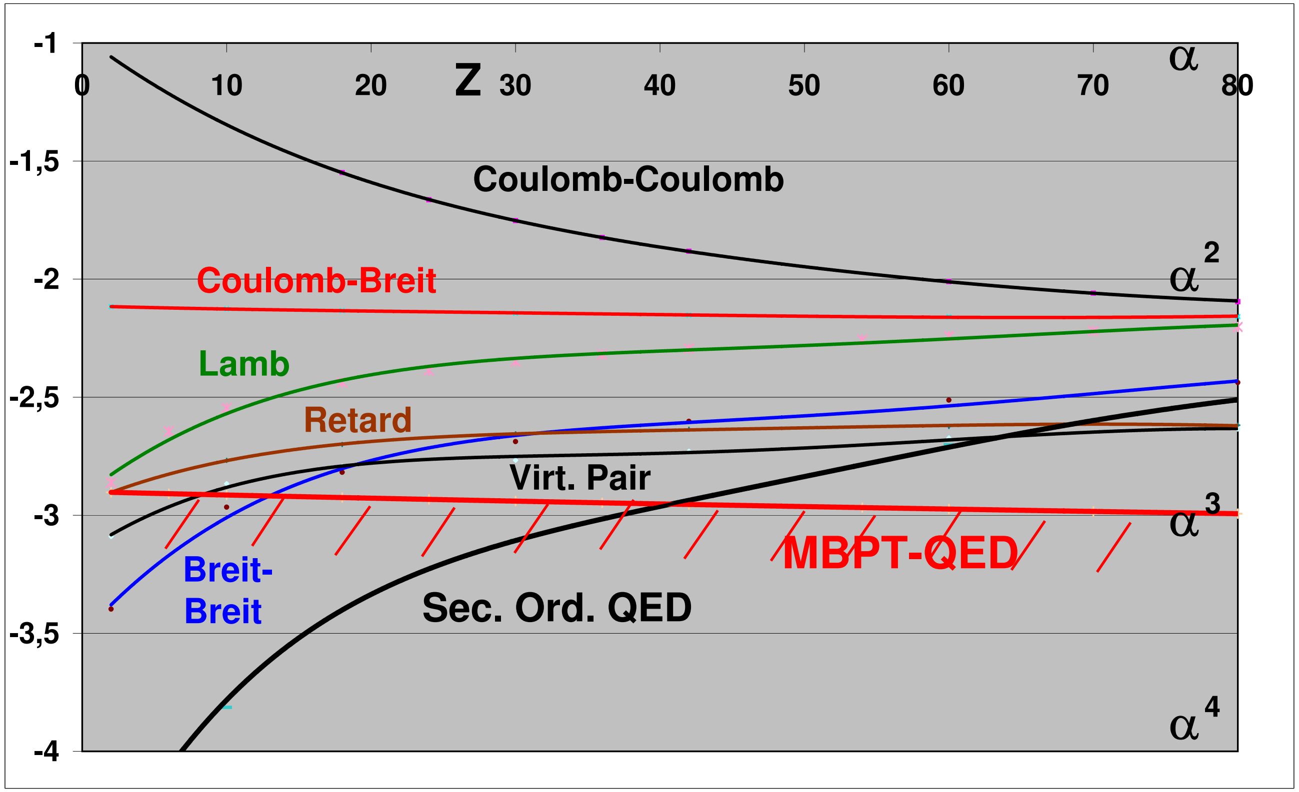
He-like Ions

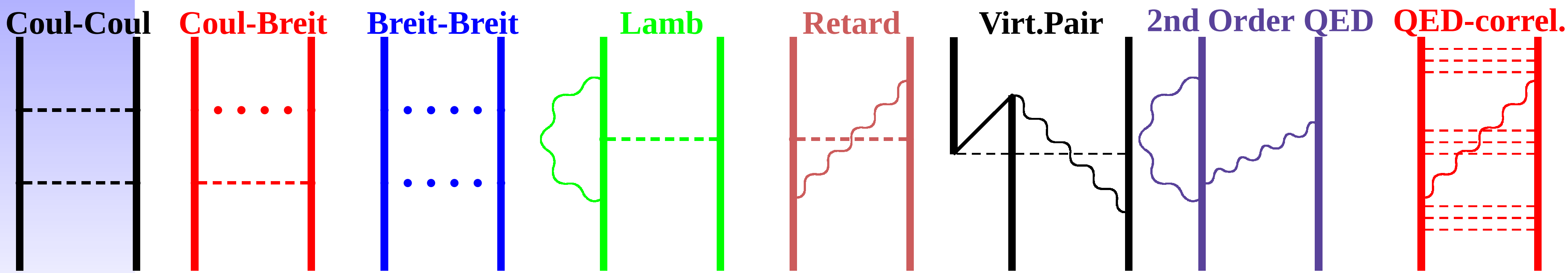
Dirac-Coulomb-Breit

1st Order QED

2nd Order QED

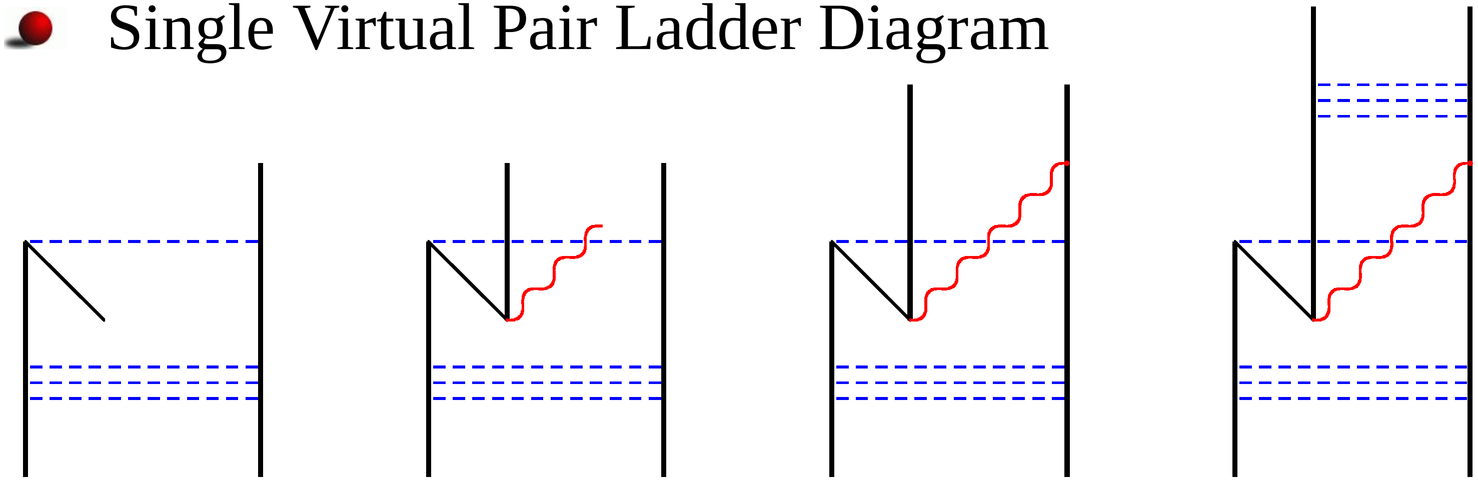
MBPT-QED





Production Line, VP

- Single Virtual Pair Ladder Diagram



(a) (b) (c) (d)

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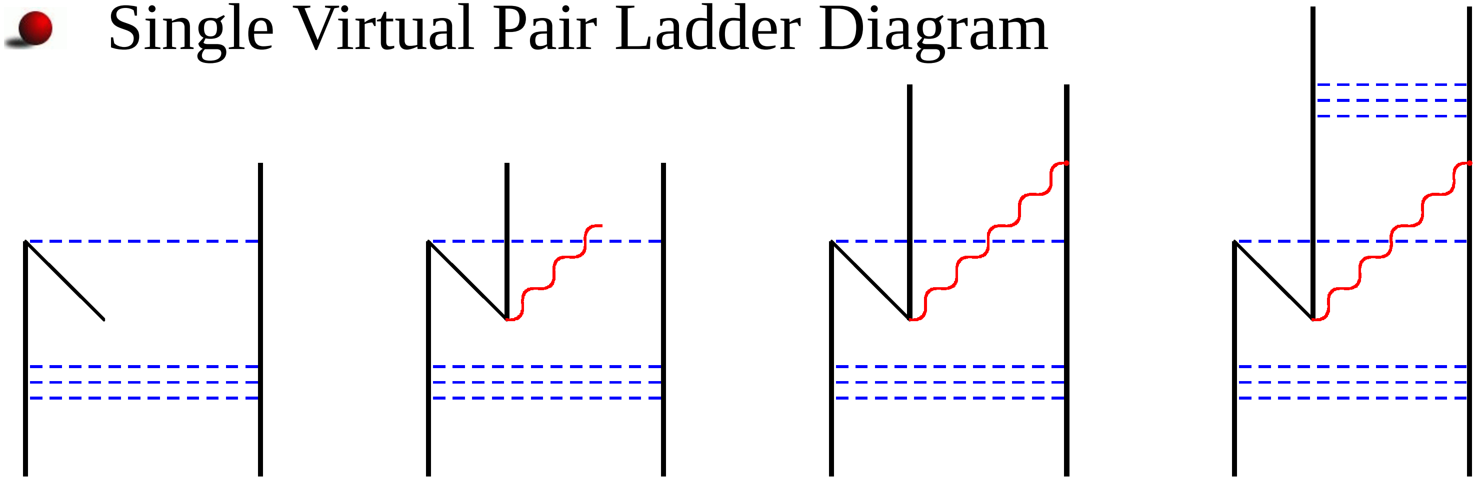

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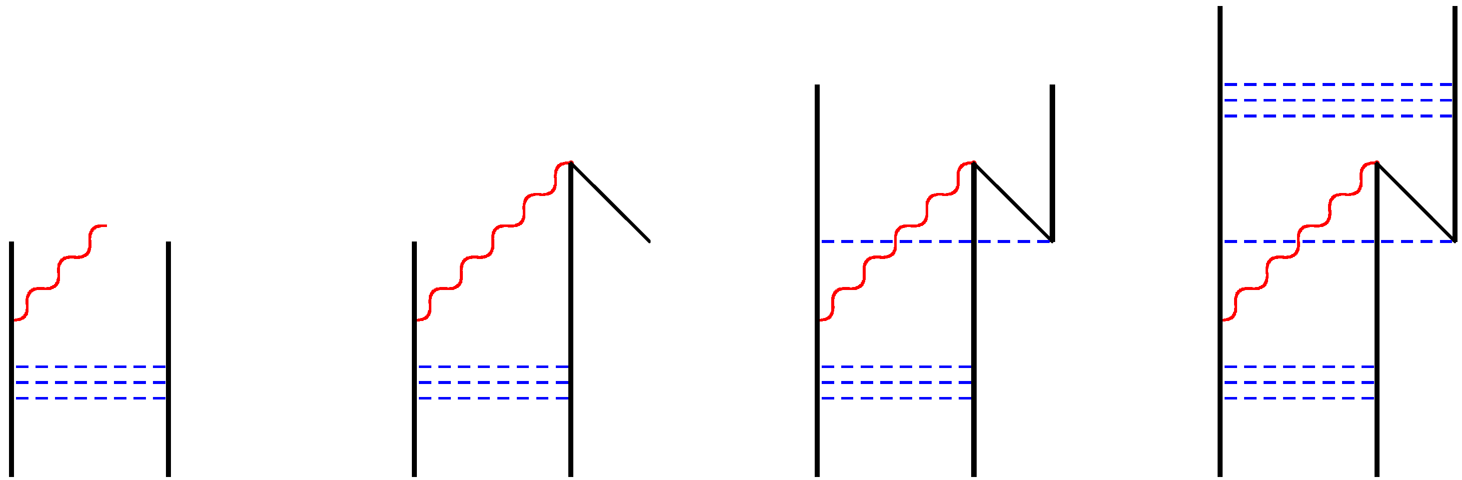

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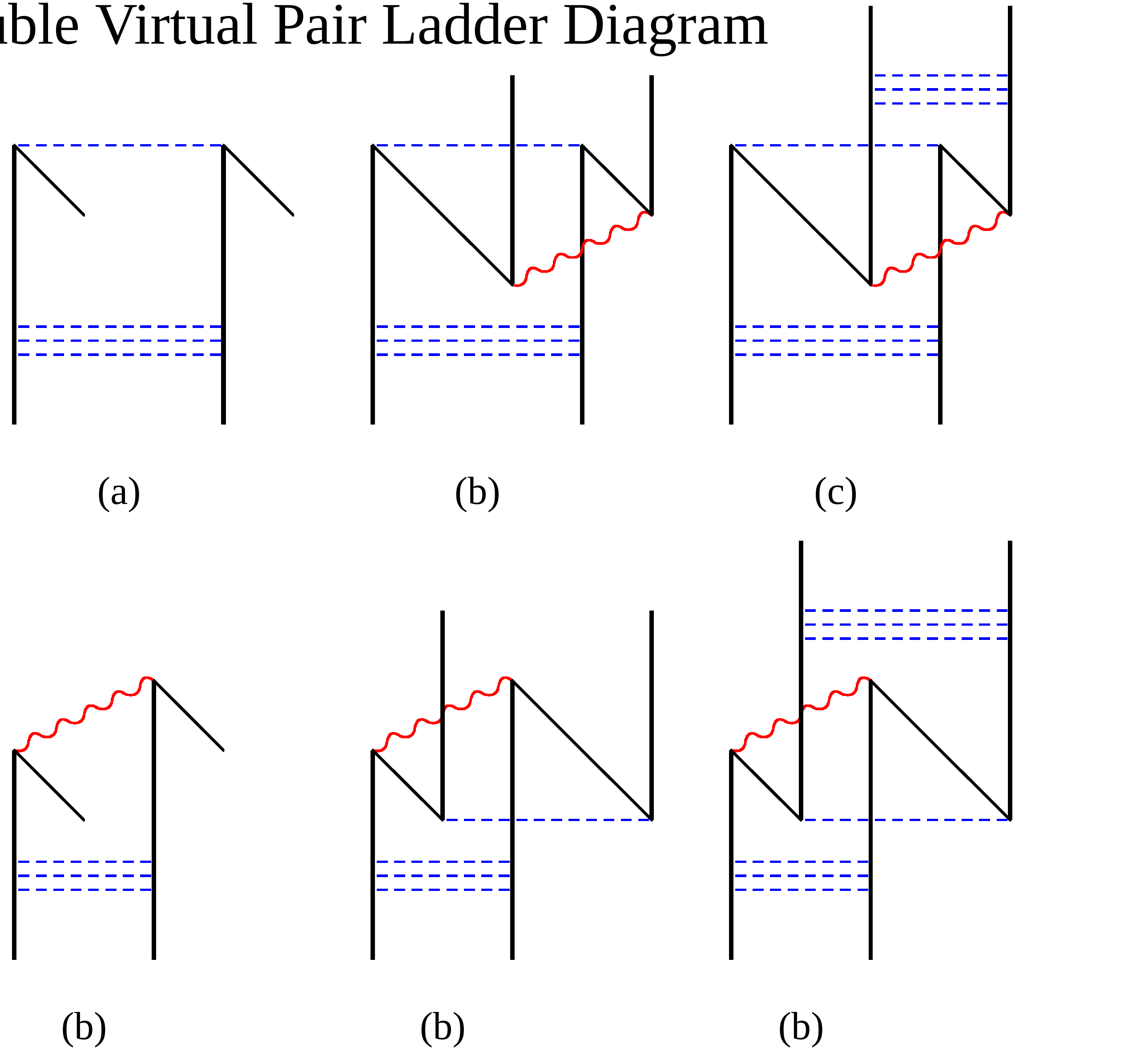
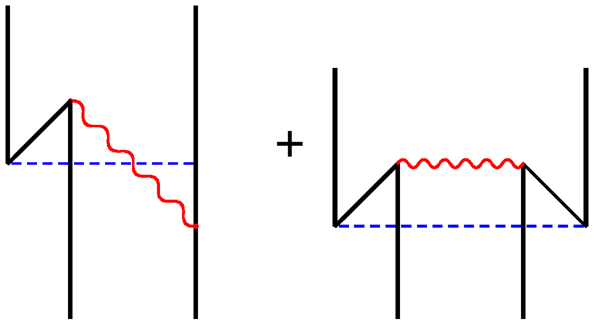


Numerical results, VP Ladder

He-like neon ground state, non-rad. effect (in μH)

Coulomb - Breit

SVP + DVP Ladder



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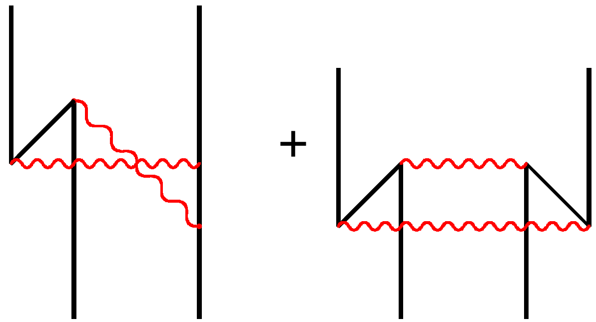
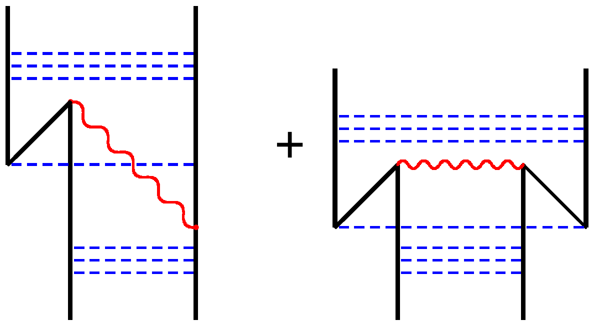
Breit - Breit

SVP + DVP Ladder



-43

+ Correlation



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Numerical results, VP Ladder

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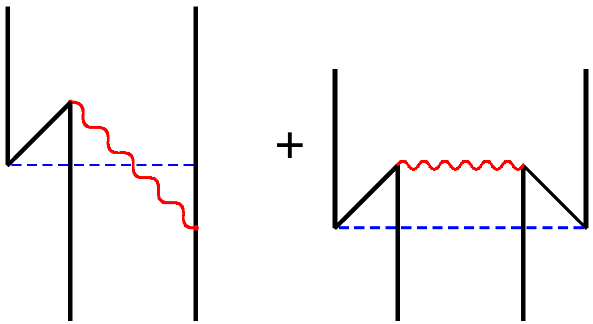

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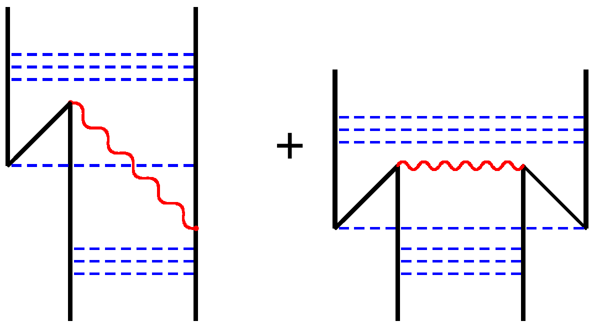

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Breit - Breit

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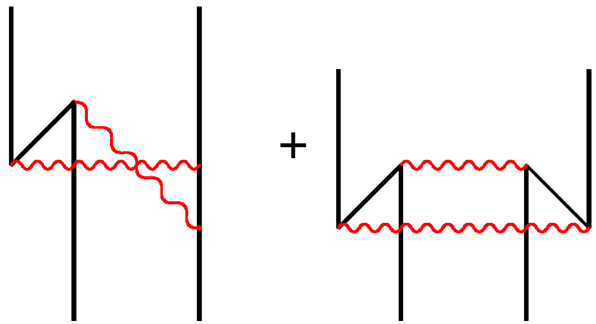

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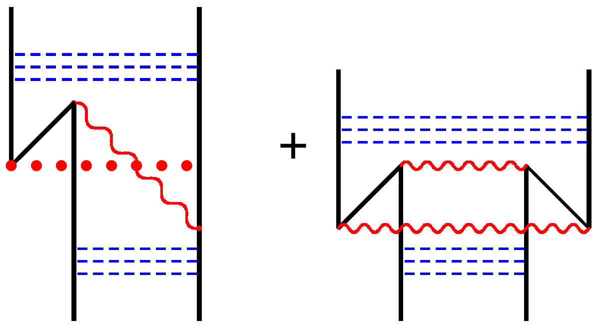
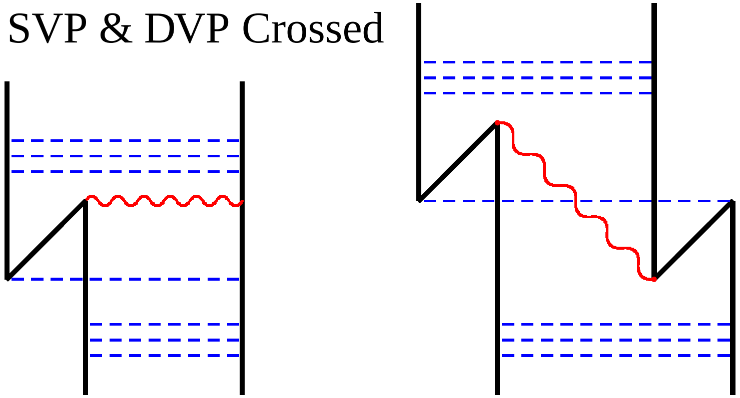


Cross Diagrams, VP

Coulomb - Breit

SVP & DVP Crossed



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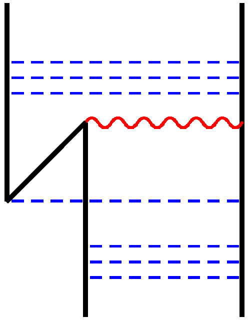

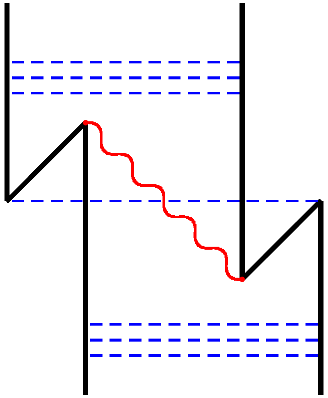

Breit - Breit

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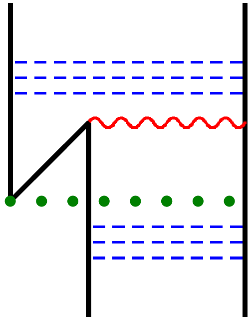

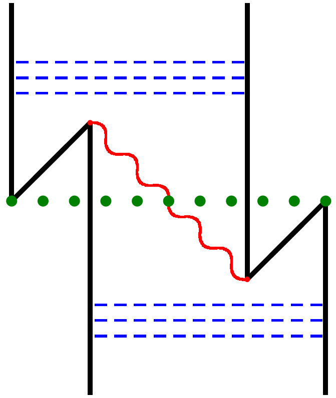

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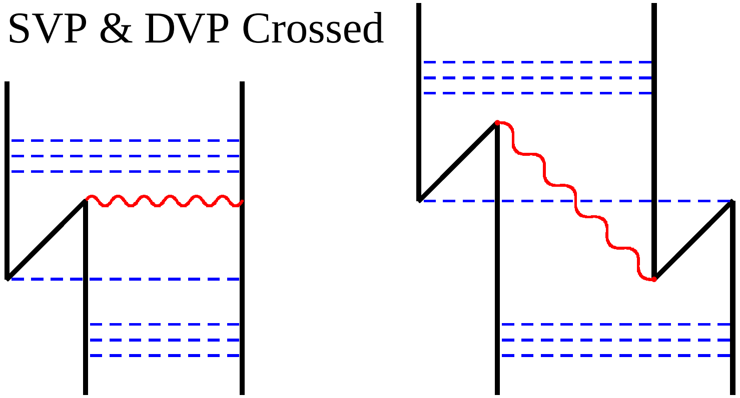
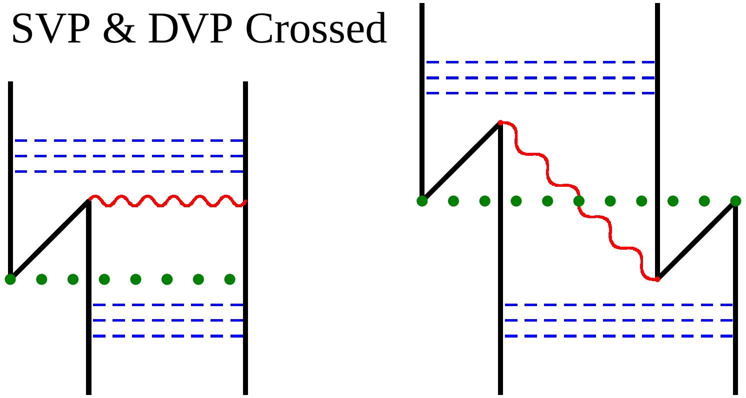


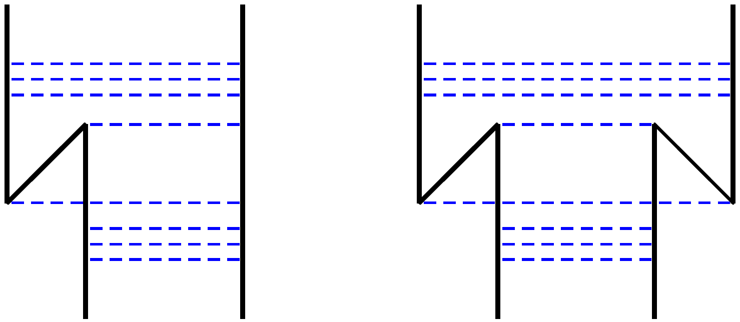
Breit - Breit

SVP & DVP Crossed



Coulomb - Coulomb

SVP & DVP



Cross Diagrams, VP

Coulomb - Breit

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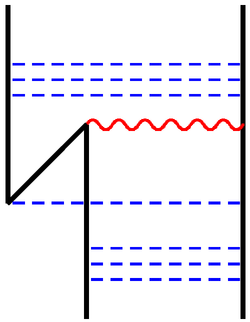
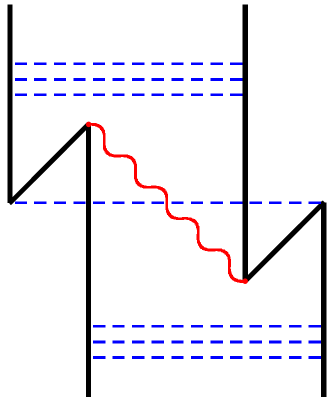
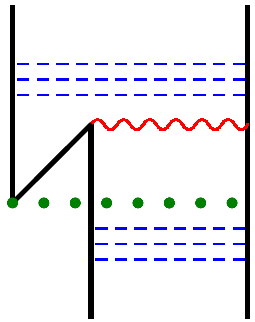
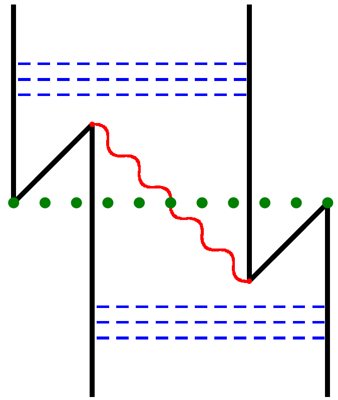




Breit - Breit

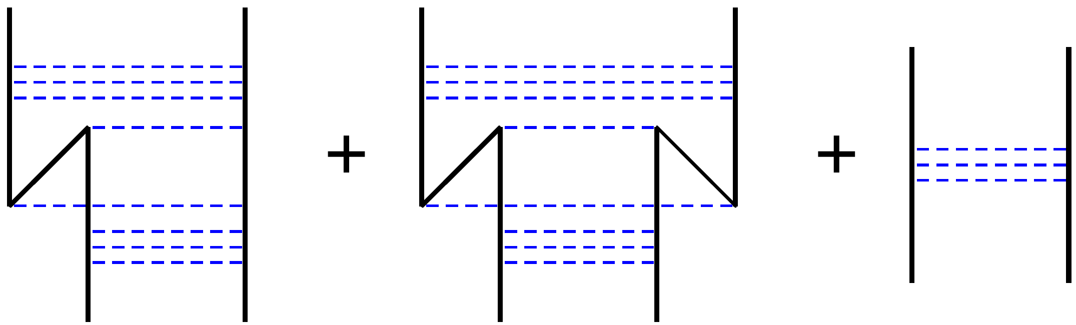
SVP & DVP Crossed



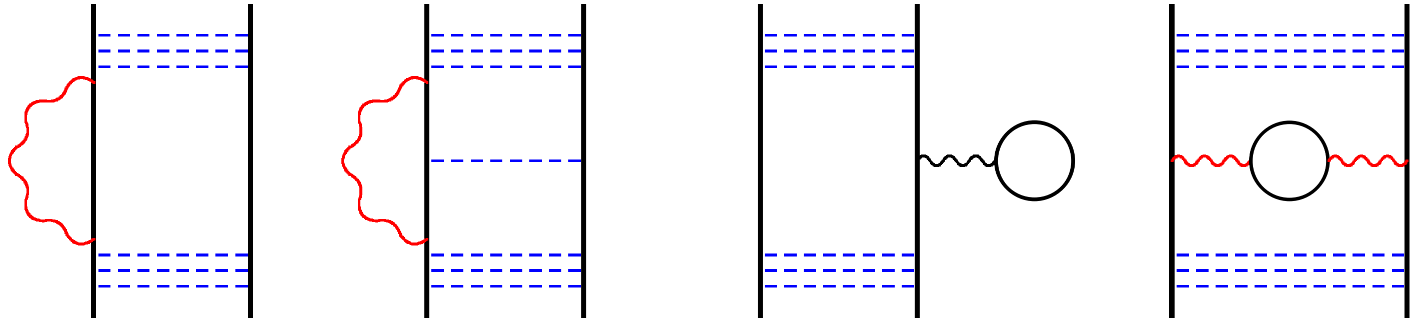


Coulomb - Coulomb

SVP & DVP

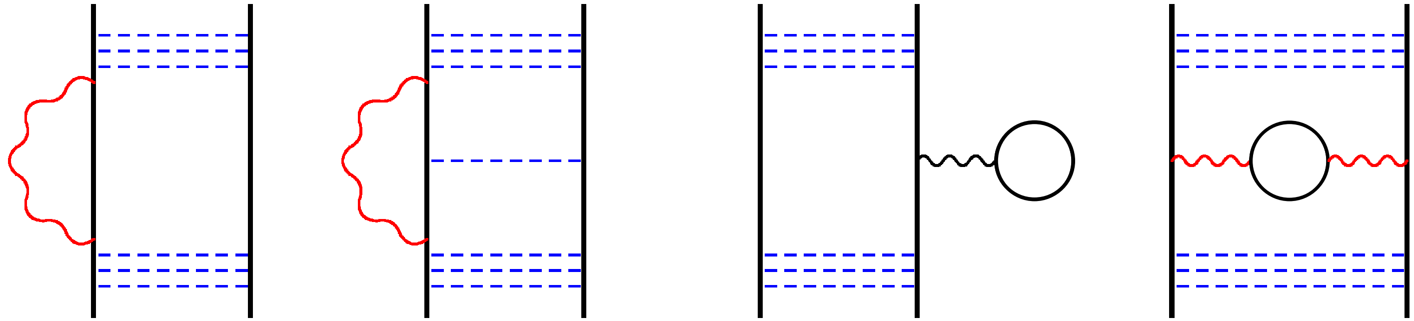


Radiative Effects

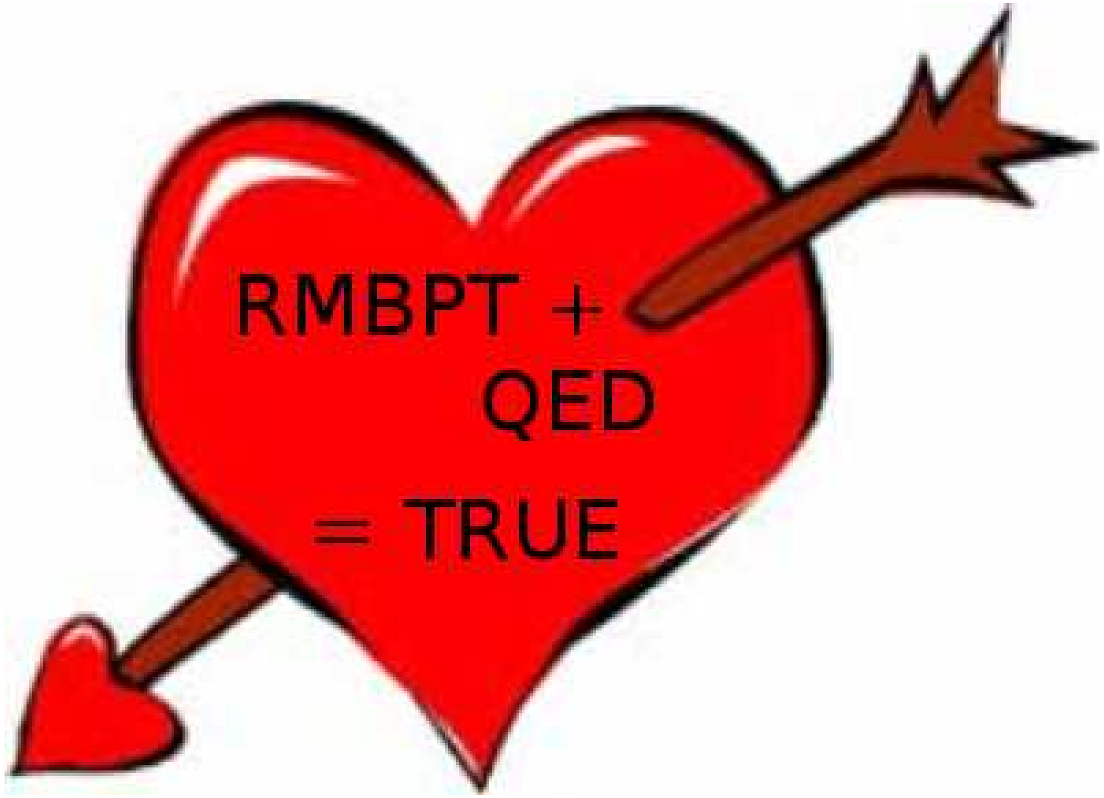


- Two approaches are under consideration
  - The Partial Wave Renormalization

Radiative Effects



- Two approaches are under consideration
  - The Partial Wave Renormalization
  - Expansion of the internal electron propagators in the nuclear Coulomb field
    - Gregory S. Adkins, Phys. Rev. D 27, 1814 - 1820 (1983)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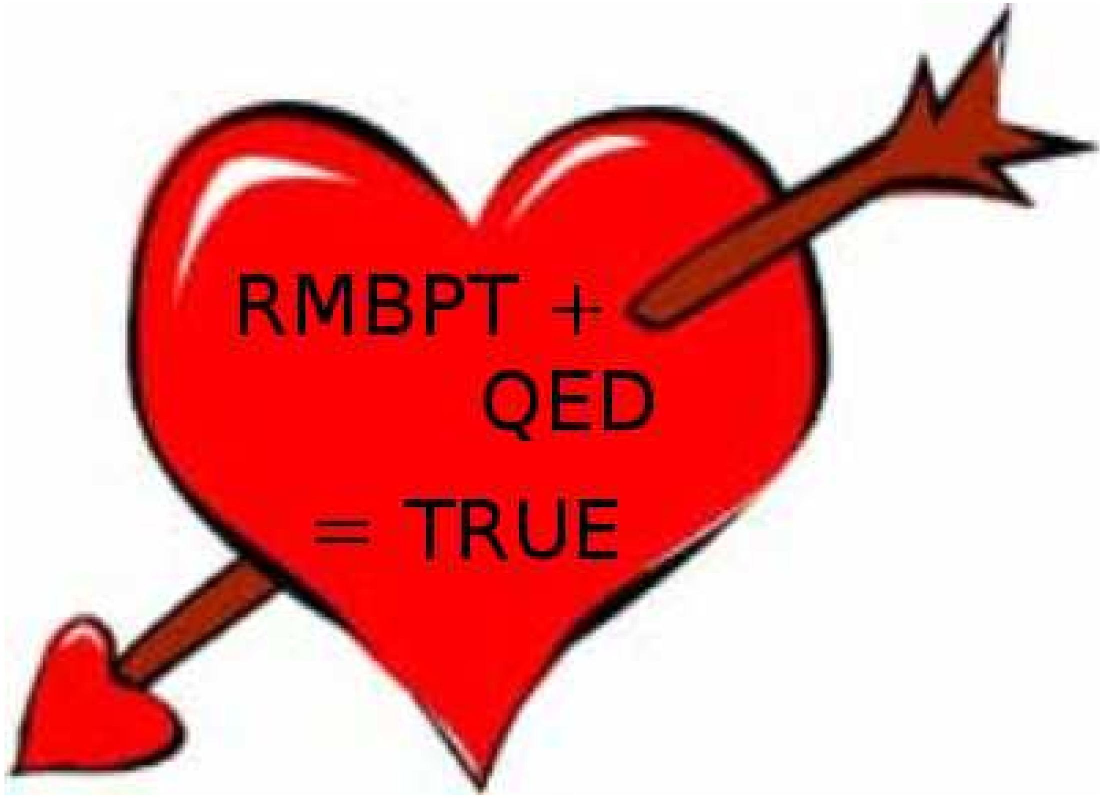

First happely married after a successful test of the radiative effects