

**Numerical Implementation of the
Relativistically Covariant
Many-Body Perturbation Theory**
A status report from the Gothenburg group

Daniel Hedendahl

Ingvar Lindgren & Sten Salomonson

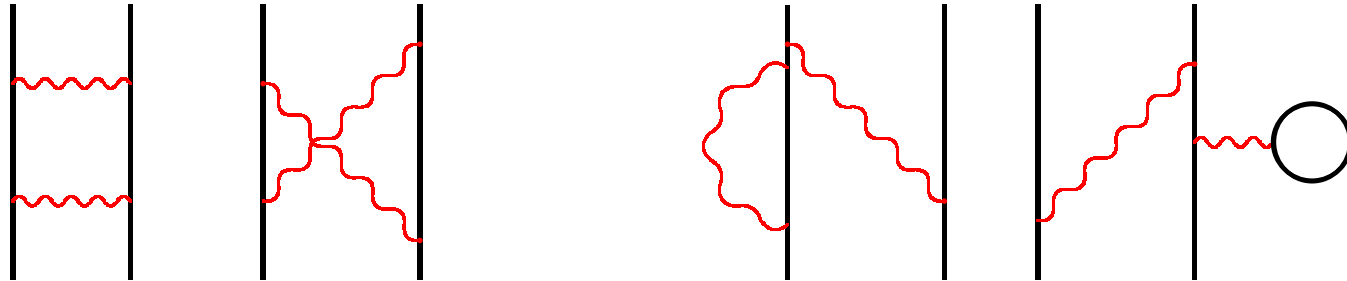
Department of physics at Göteborg University, Göteborg,
Sweden

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



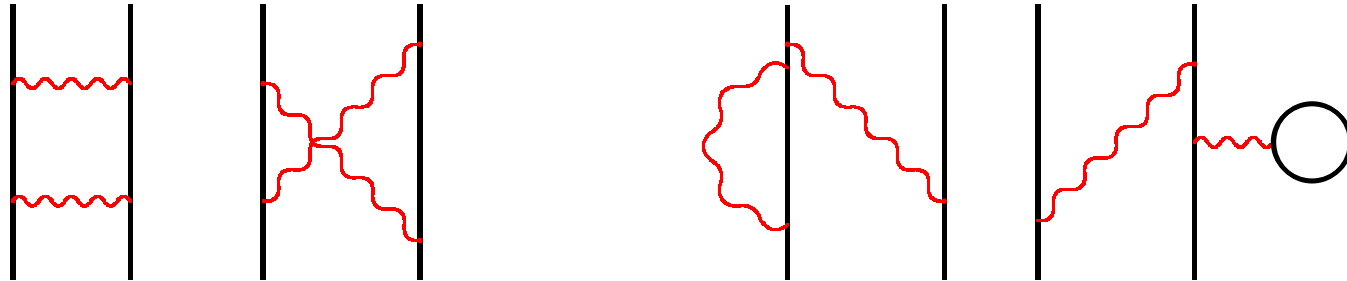
Photon Exchange

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.

● The Two-Photon Effects



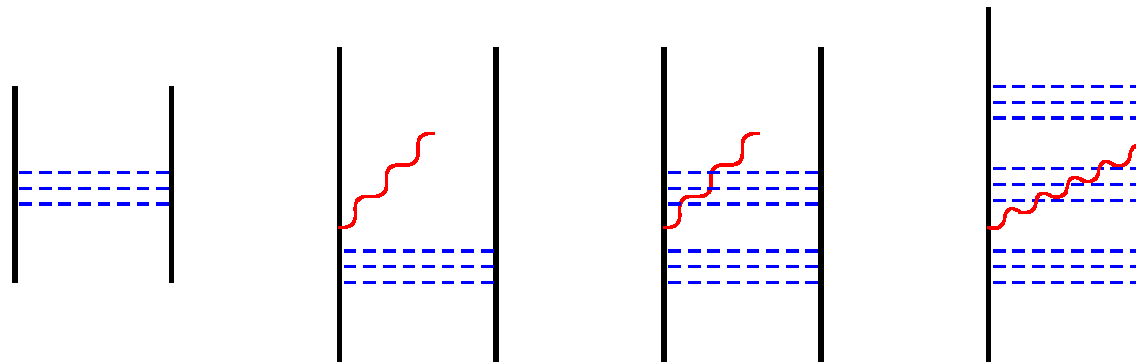
Photon Exchange

Radiative Effects

● B. Åsén *et al.*, Phys. Rev. A 65, 032516 (2002)

● A.N. Artemyev *et al.*, Phys. Rev. A 71, 062104 (2005)

● 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

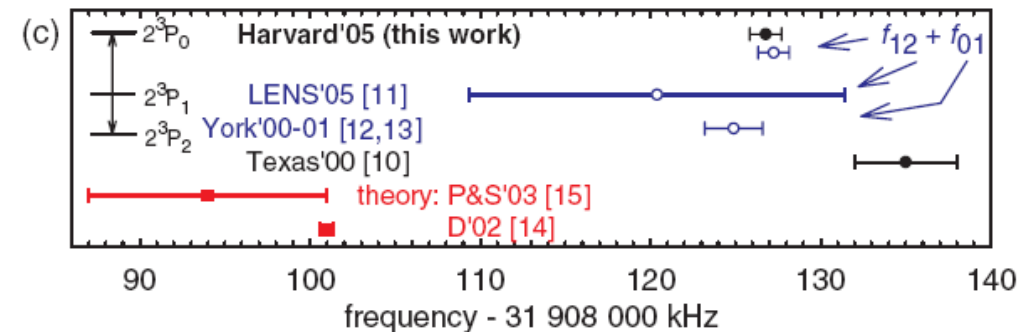
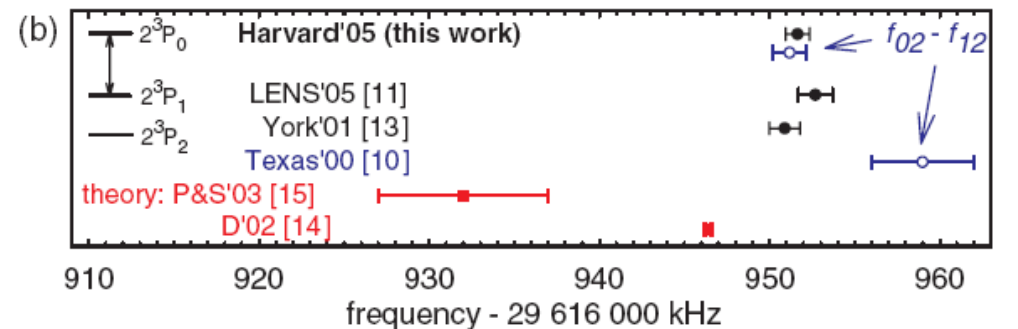
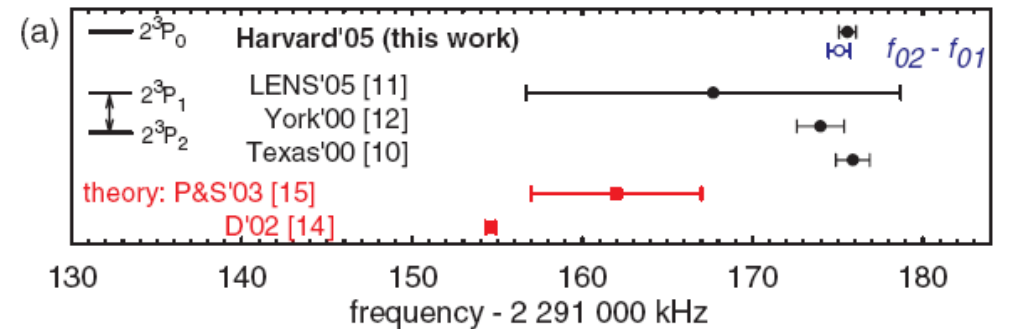
Independent determination of the fine-structure constant α

Experimental values,

- G. Gabrielse *et al.*,
Harvard
- E.A. Hessels *et al.*, York
- M. Inguscio *et al.*,
LENS
- J. Castilleja *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-Degeneracy
 - Extended Model Space
 - $P + Q = 1$
- Generalized Bloch equation

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

Std Relativistic MBPT

- Dirac-Coulomb Approximation

$$H = \Lambda_+ \left[\sum_{i=1}^N h_D(i) + \sum_{i<j}^N \frac{e^2}{4\pi r_{ij}} \right] \Lambda_+$$

Std Relativistic MBPT

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- Dirac-Coulomb-Breit Approximation

$$H = \Lambda_+ \left[\sum_{i=1}^N h_D(i) + \sum_{i<j}^N \frac{e^2}{4\pi r_{ij}} + H_B \right] \Lambda_+$$

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

Std Relativistic MBPT

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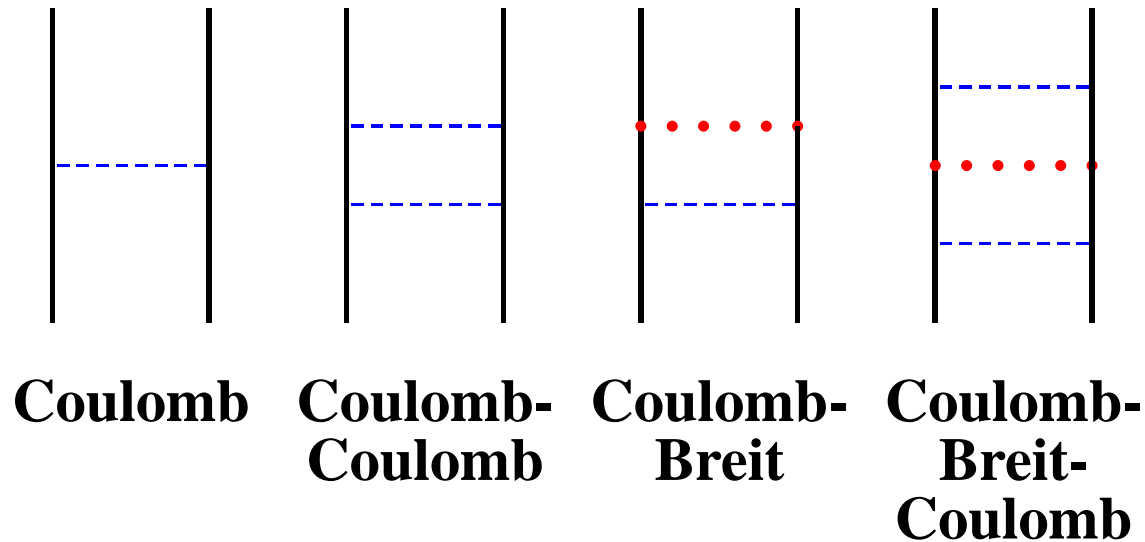
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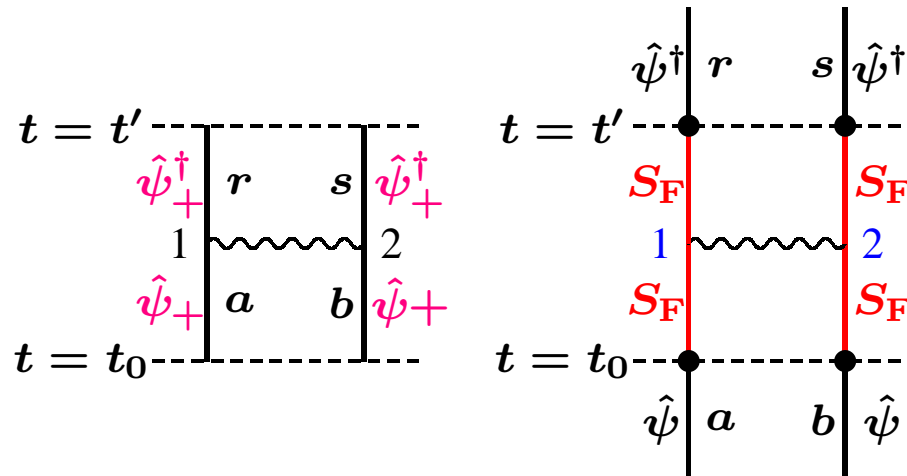
$$H_B = -\frac{e^2}{8\pi} \sum_{i<j} \left[\frac{\alpha_i \cdot \alpha_j}{r_{ij}} + \frac{(\alpha_i \cdot r_{ij})(\alpha_j \cdot r_{ij})}{r_{ij}^3} \right]$$

- 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**

$$\begin{aligned}
 U_{\text{Cov}}^{(2)}(t', -\infty) &= -\frac{1}{2} \iint d^3x'_1 d^3x'_2 \hat{\psi}^\dagger(x'_1) \hat{\psi}^\dagger(x'_2) \\
 &\times \iint d^4x_1 d^4x_2 G_0(x'_1, x'_2; x_1, x_2) \iint d^3x'_{10} d^3x'_{20} iI(x_1, x_2) \\
 &\times G_0(x_1, x_2; x_{10}, x_{20}) \hat{\psi}(x_{10}) \hat{\psi}(x_{20}) e^{-\gamma(|t_1| + |t_2|)}
 \end{aligned}$$

- Integration of t_1 and t_2 is performed over all time

C.E.O. Method

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

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

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

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

- 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

$$[\Omega_I, H_0]P = V_{12}\Omega_I P - \Omega_I P \cdot V_{\text{eff}}$$

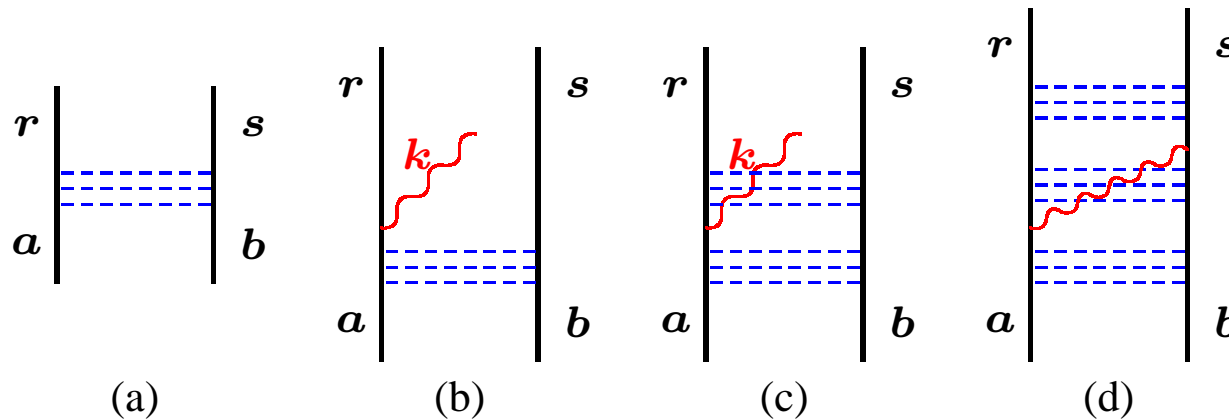
- Bloch equation with an "uncontracted" photon

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

- Bloch equation with a "contracted" photon

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

Our Production Line, NVP



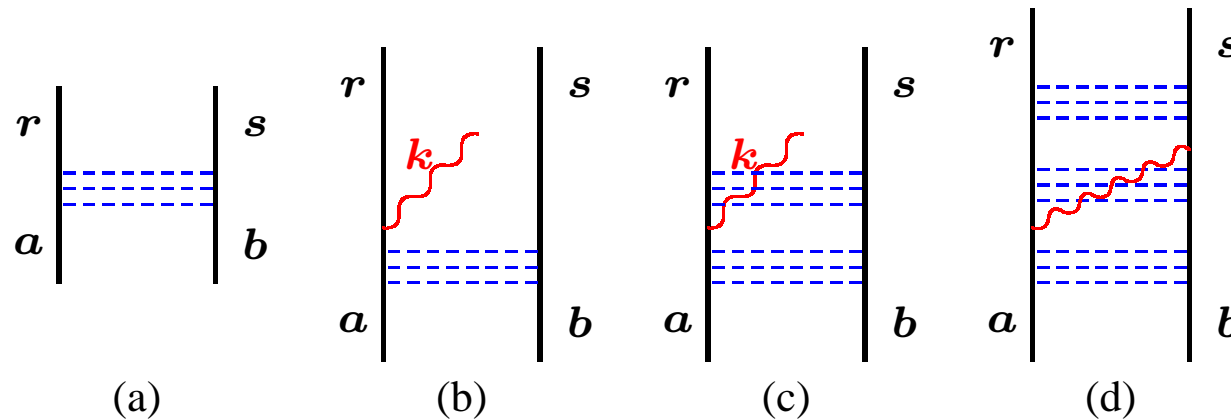
- Instantaneous Coulomb interactions, V_{12} (a)

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

- One retarded interaction (b)

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

Our Production Line, NVP



- Crossing Coulomb interactions (c)

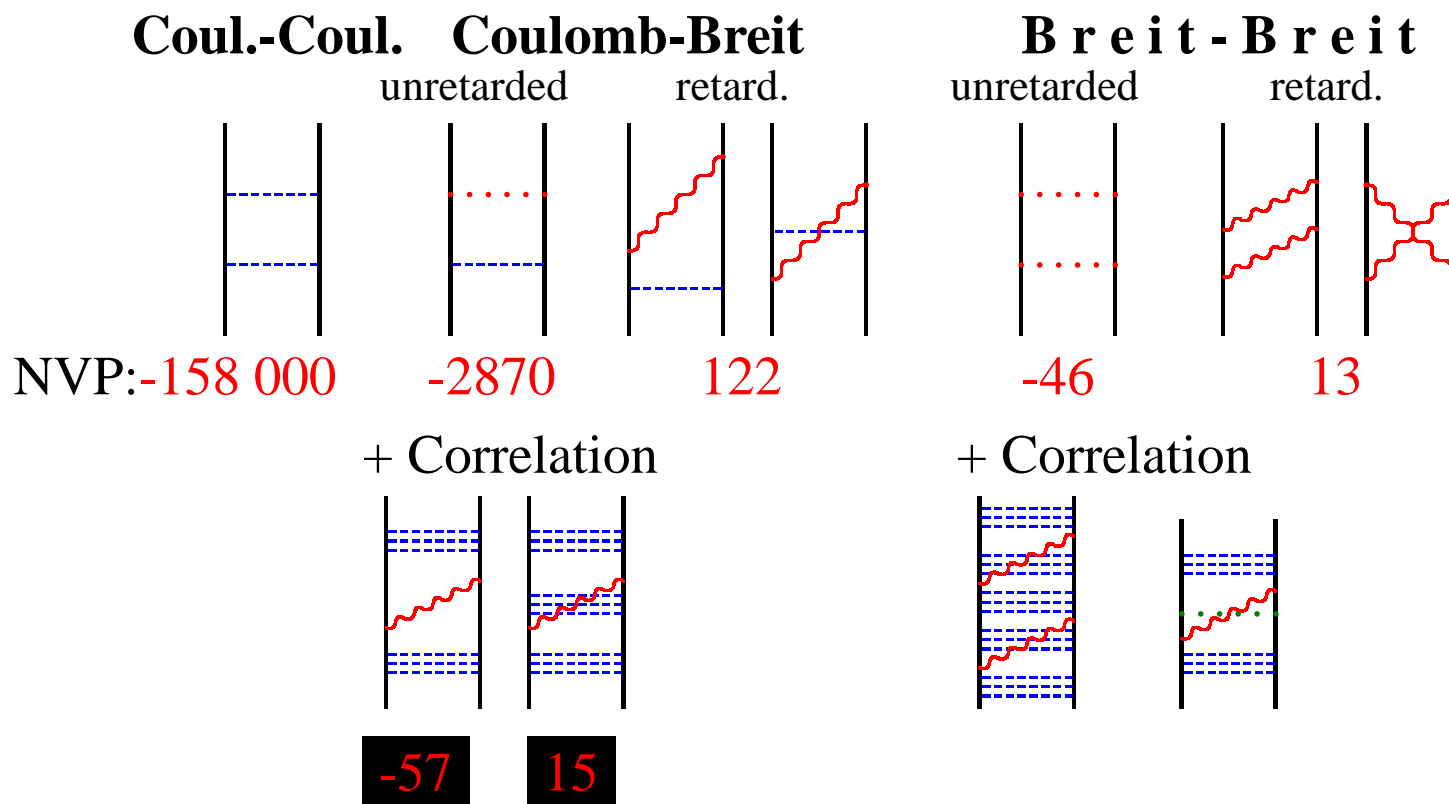
$$\begin{aligned}
 (\mathcal{E} - H_0 - k) |\rho_{ab}^l(k)\rangle &= |rs\rangle \langle rs| V^l(k) |\rho_{ab}\rangle \\
 &+ |rs\rangle \langle rs| V_{12} |\rho_{ab}^l(k)\rangle - |\rho_{cd}^l(k)\rangle \langle cd| V_{\text{eff}} |ab\rangle
 \end{aligned}$$

- Absorbing photon, additional Coulomb interactions (d)

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

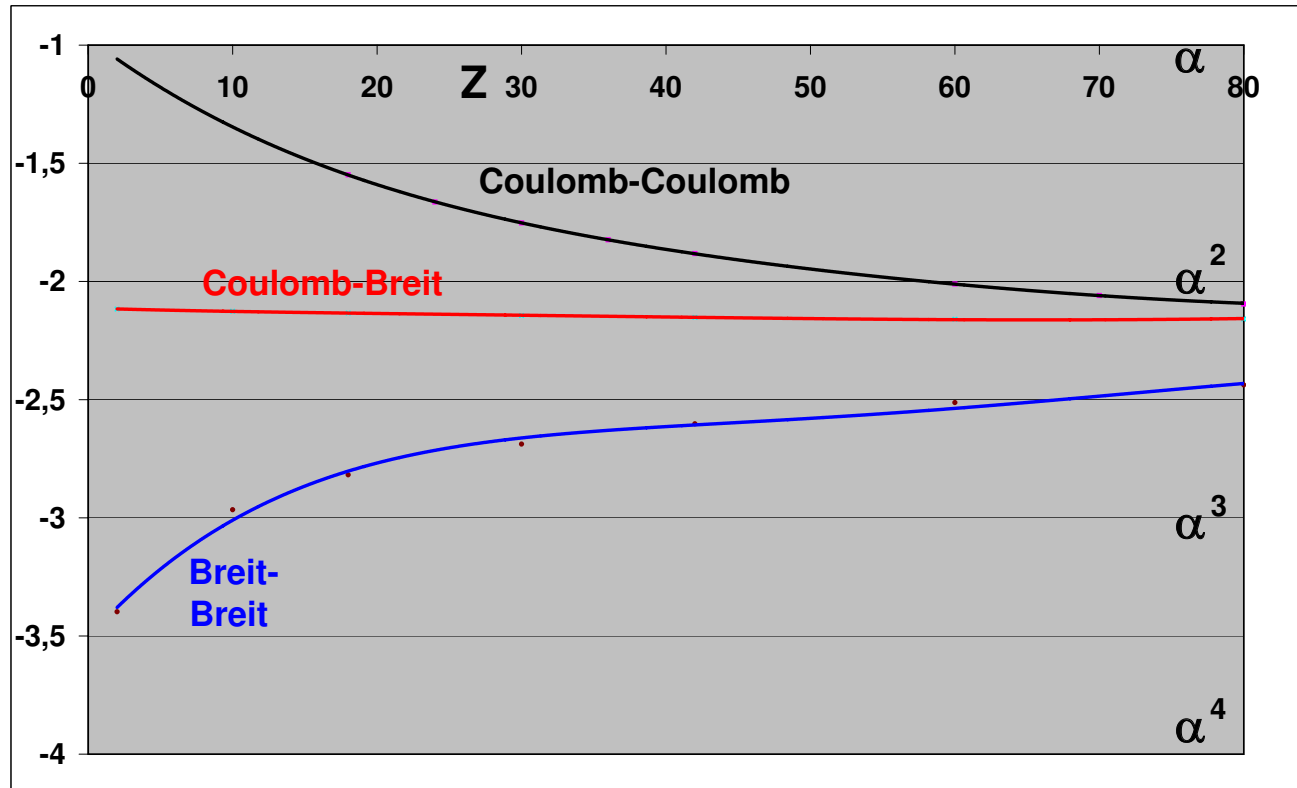
Numerical results

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



He-like Ions

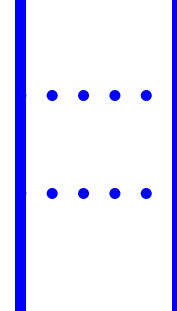
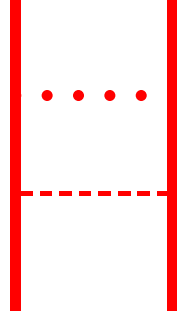
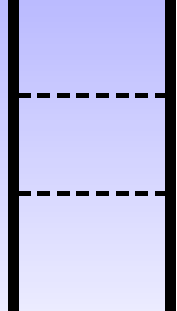
Dirac-Coulomb-Breit



Coul-Coul

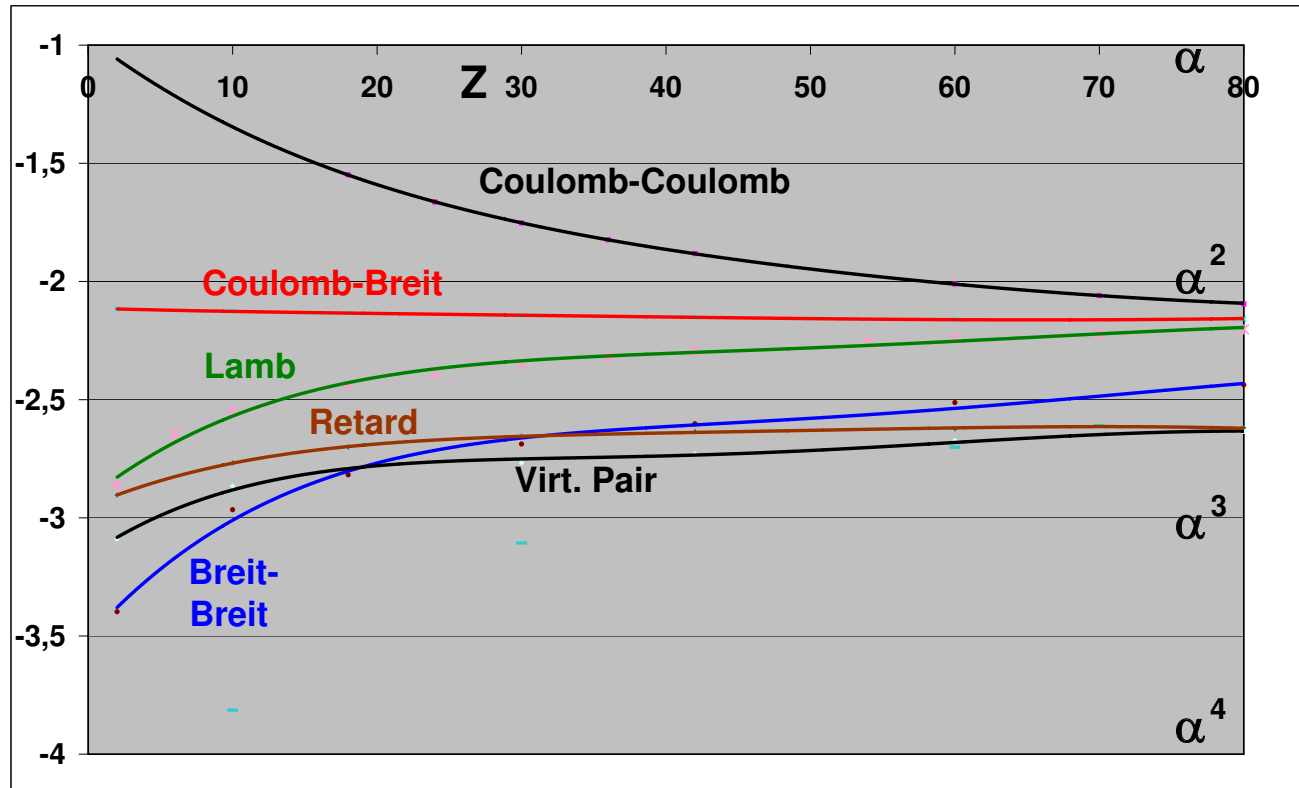
Coul-Breit

Breit-Breit

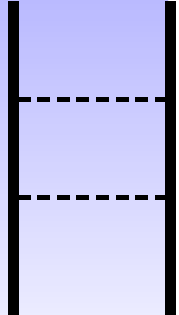


He-like Ions

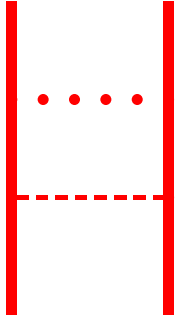
Dirac-Coulomb-Breit
1st Order QED



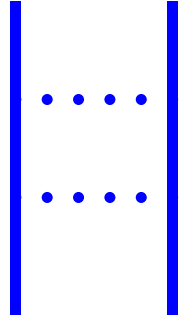
Coul-Coul



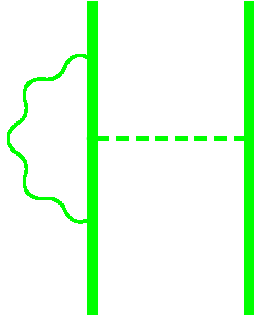
Coul-Breit



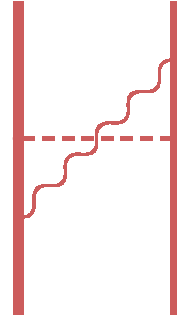
Breit-Breit



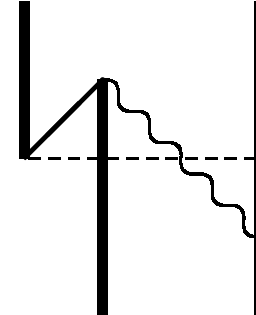
Lamb



Retard

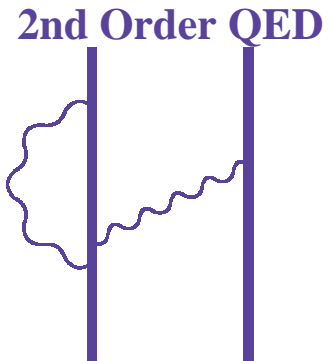
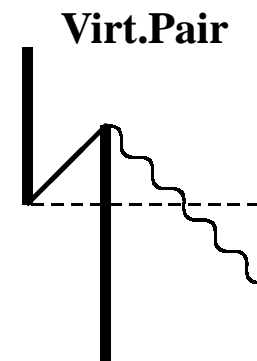
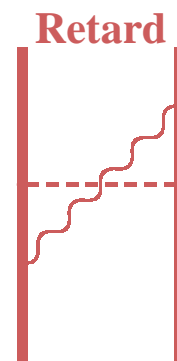
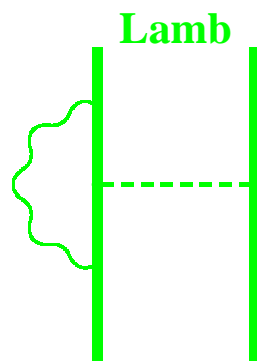
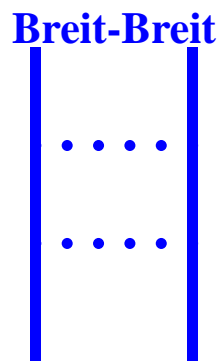
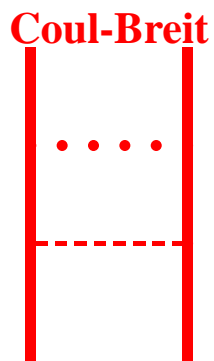
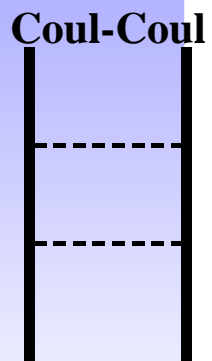
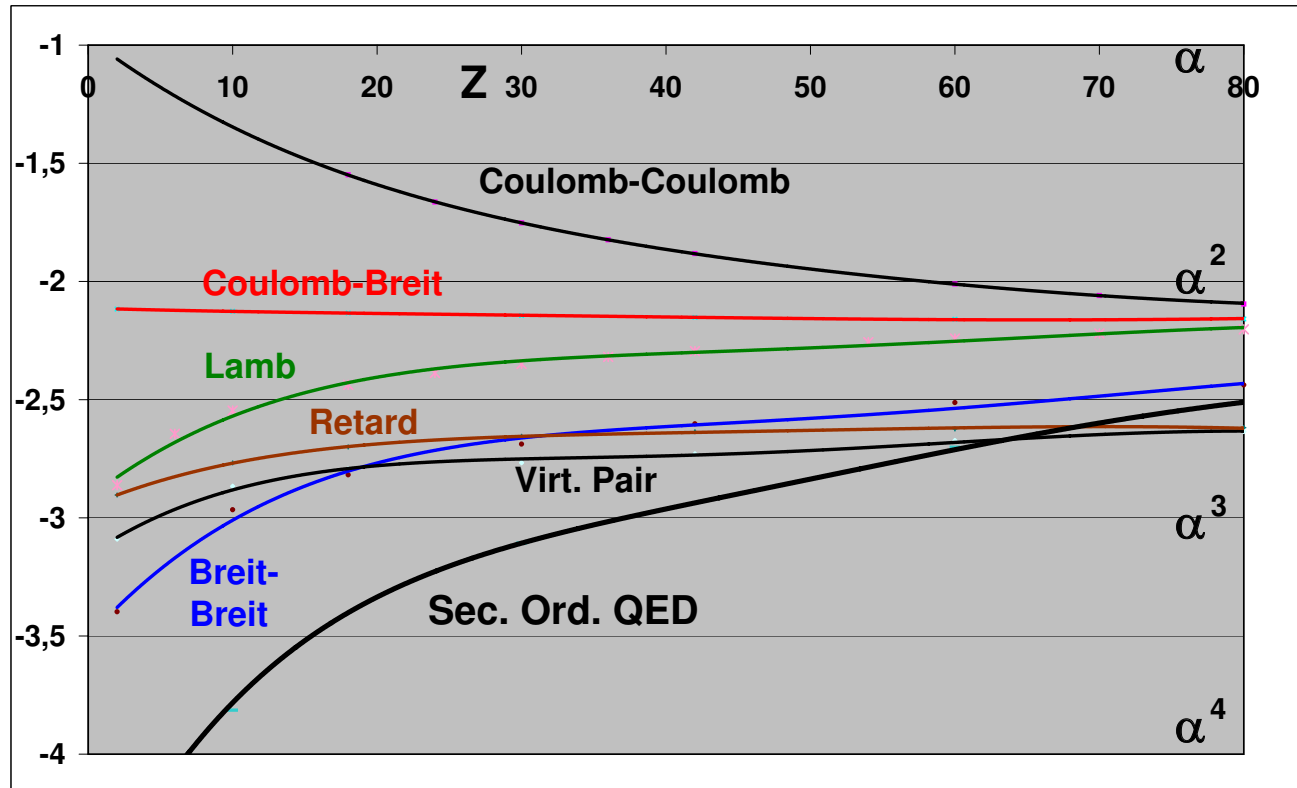


Virt.Pair



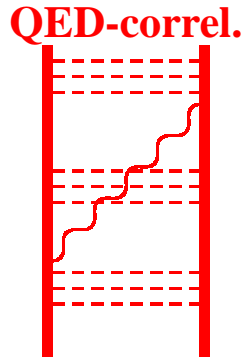
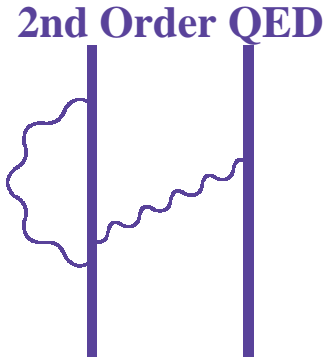
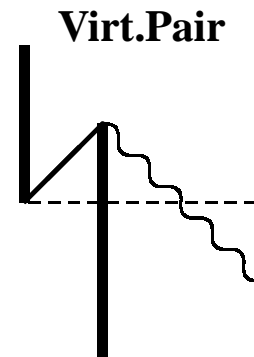
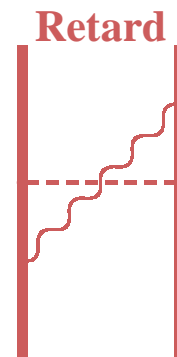
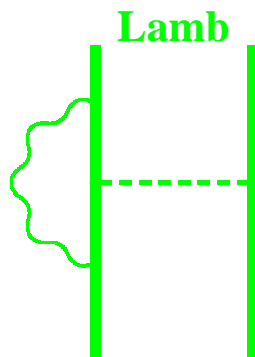
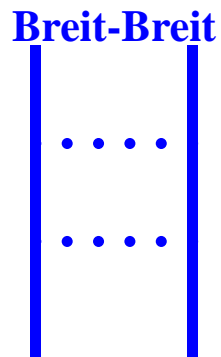
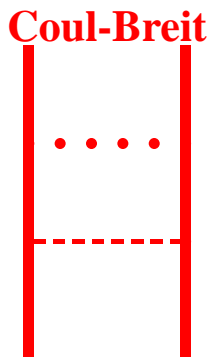
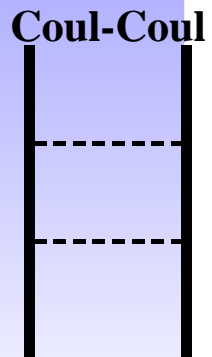
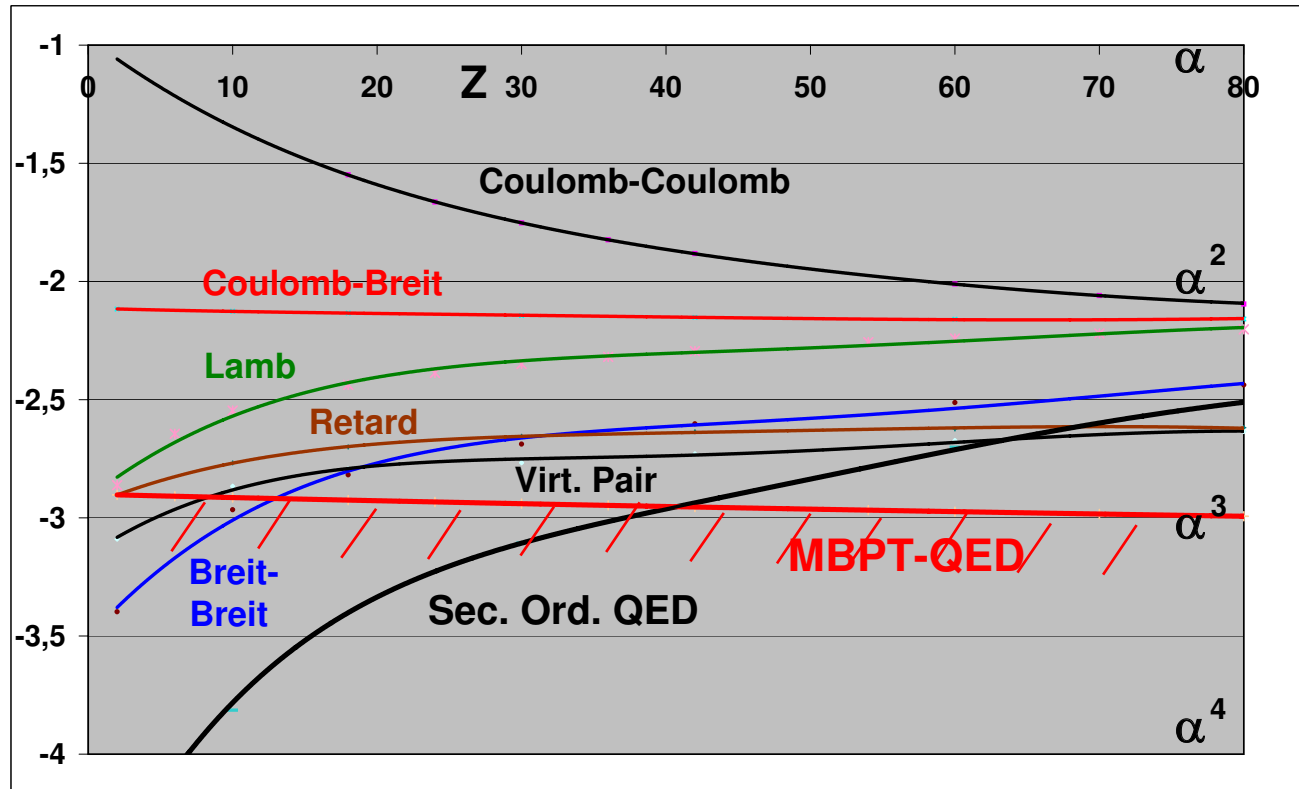
He-like Ions

Dirac-Coulomb-Breit
 1st Order QED
 2nd Order QED



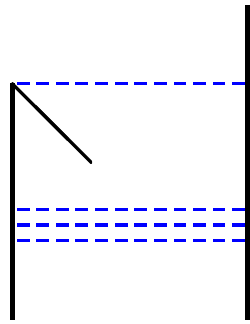
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Dirac-Coulomb-Breit
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 2nd Order QED
 MBPT-QED

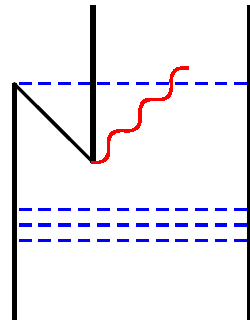


Production Line, VP

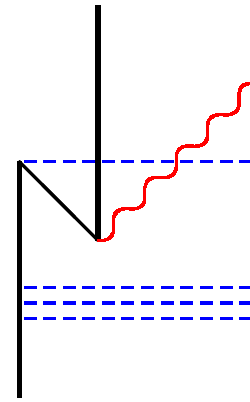
● Single Virtual Pair Ladder Diagram



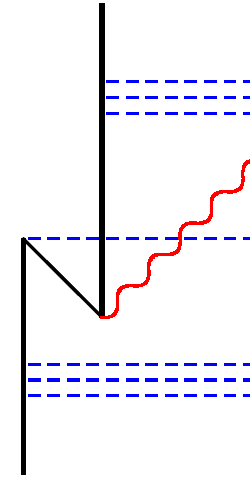
(a)



(b)



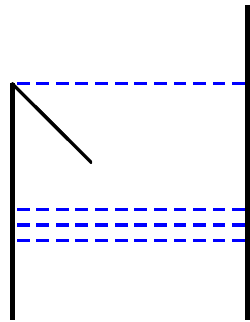
(c)



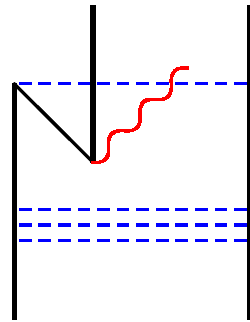
(d)

Production Line, VP

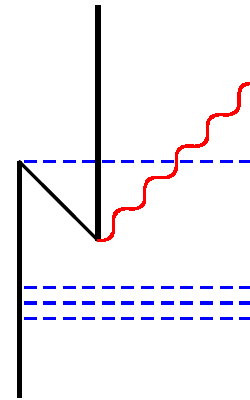
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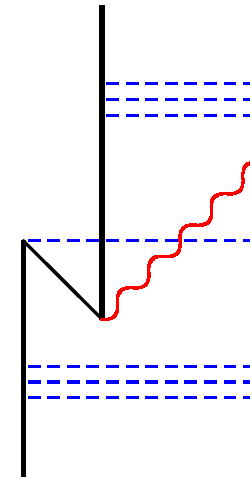
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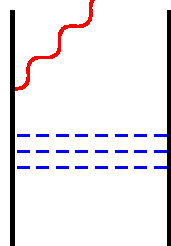
(b)



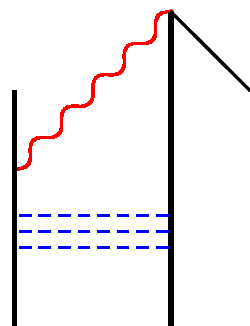
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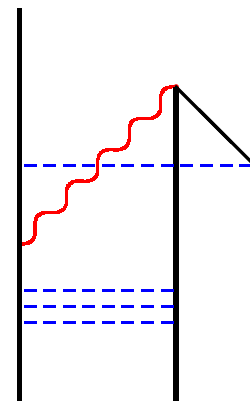
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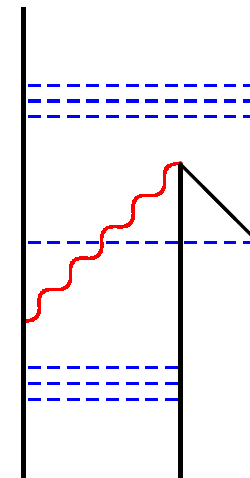
(a)



(b)



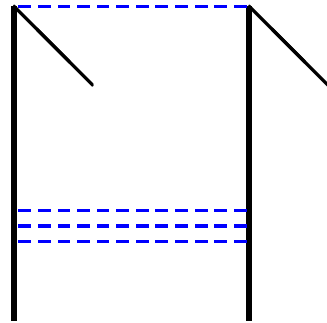
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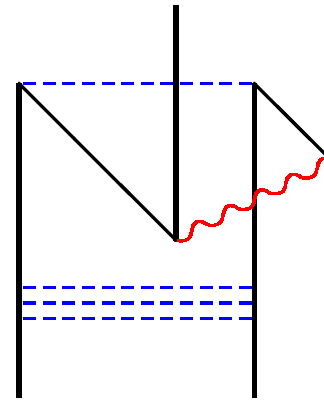
(d)

Production Line, VP

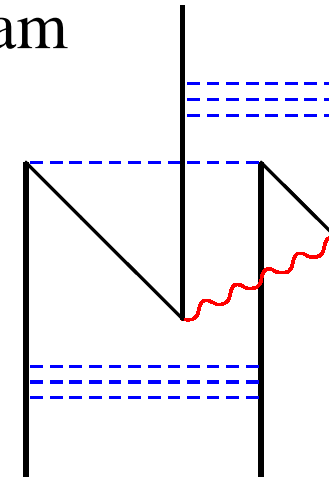
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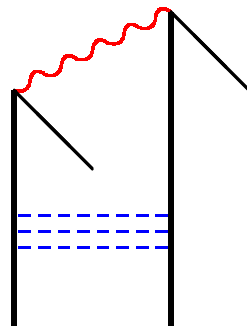
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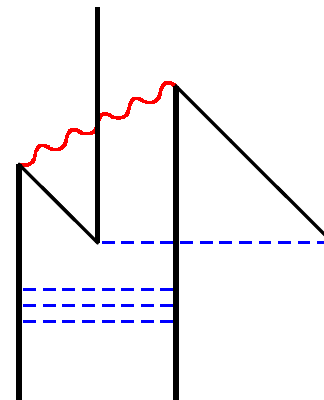
(b)



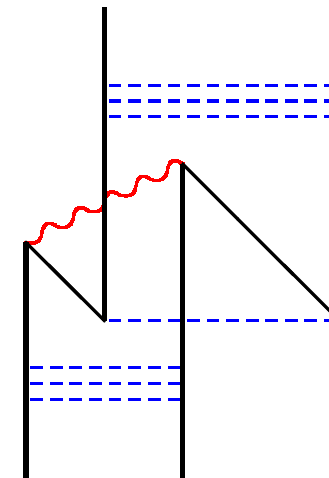
(c)



(b)



(b)



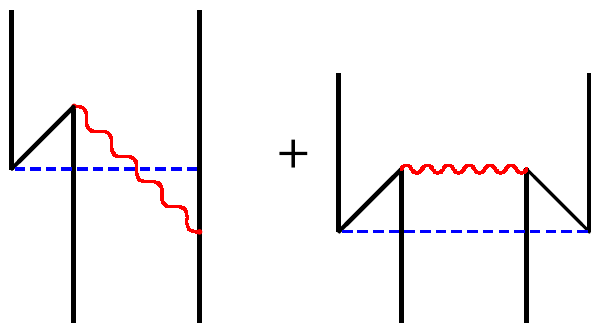
(b)

Numerical results, VP Ladder

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

Coulomb - Breit

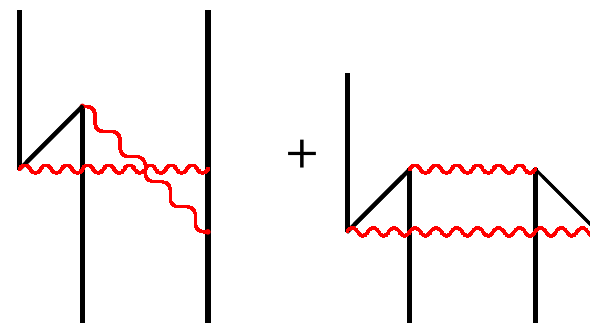
SVP + DVP Ladder



-46

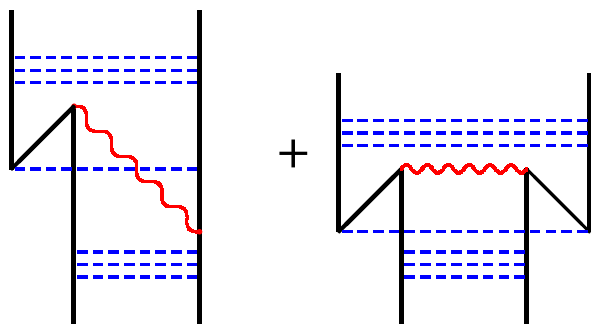
Breit - Breit

SVP + DVP Ladder



-43

+ Correlation



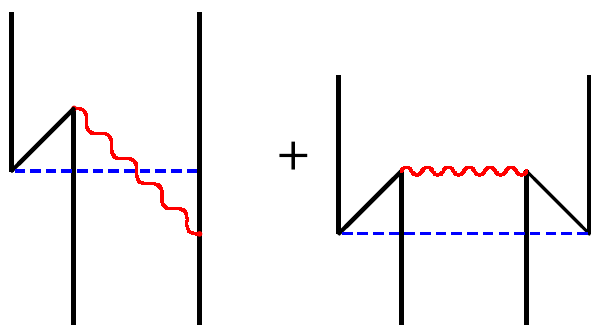
7

Numerical results, VP Ladder

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

Coulomb - Breit

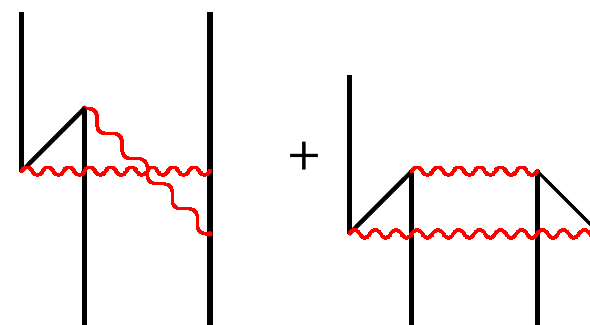
SVP + DVP Ladder



-46

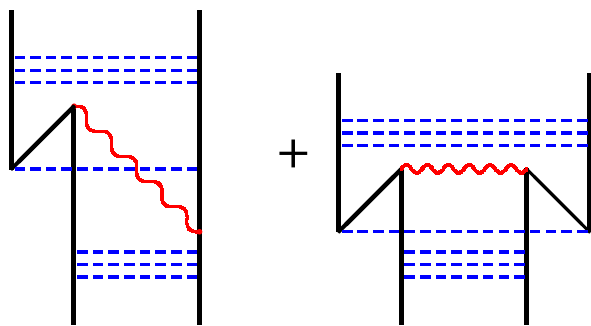
Breit - Breit

SVP + DVP Ladder

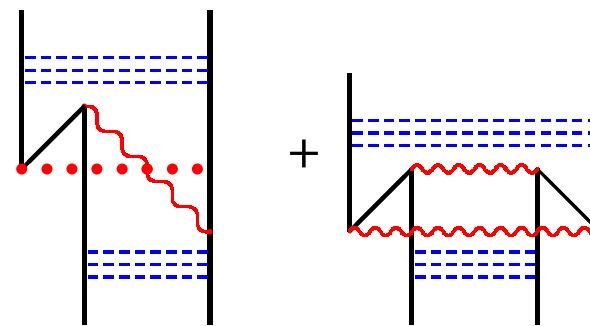


-43

+ Correlation



+ Correlation

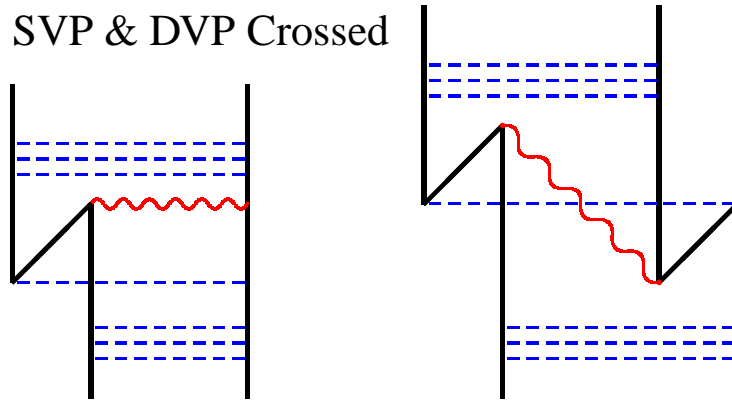


7

Cross Diagrams, VP

Coulomb - Breit

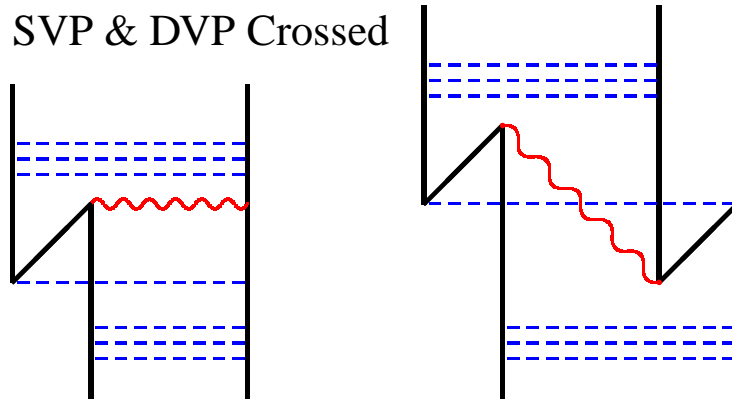
SVP & DVP Crossed



Cross Diagrams, VP

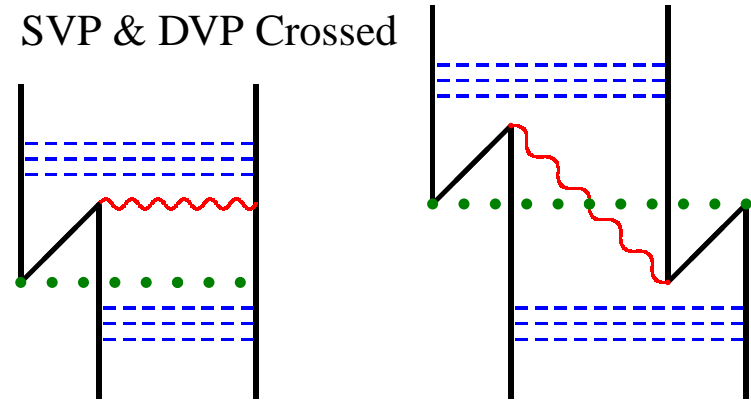
Coulomb - Breit

SVP & DVP Crossed



Breit - Breit

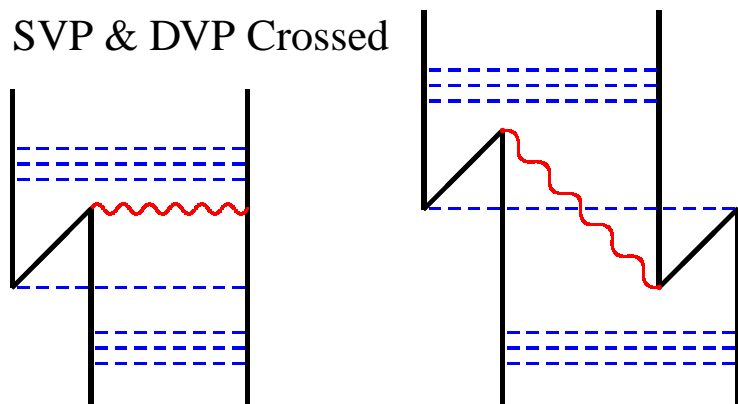
SVP & DVP Crossed



Cross Diagrams, VP

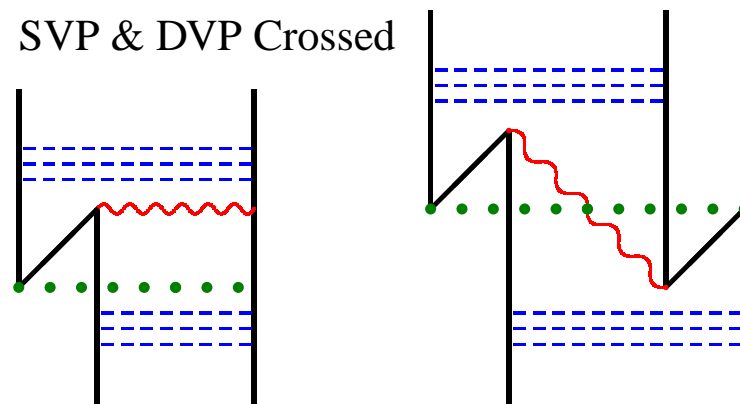
Coulomb - Breit

SVP & DVP Crossed



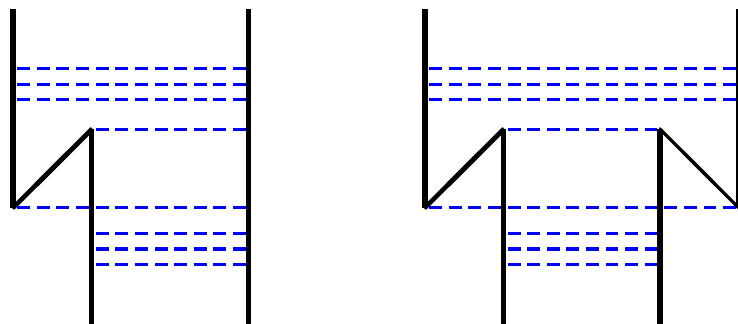
Breit - Breit

SVP & DVP Crossed



Coulomb - Coulomb

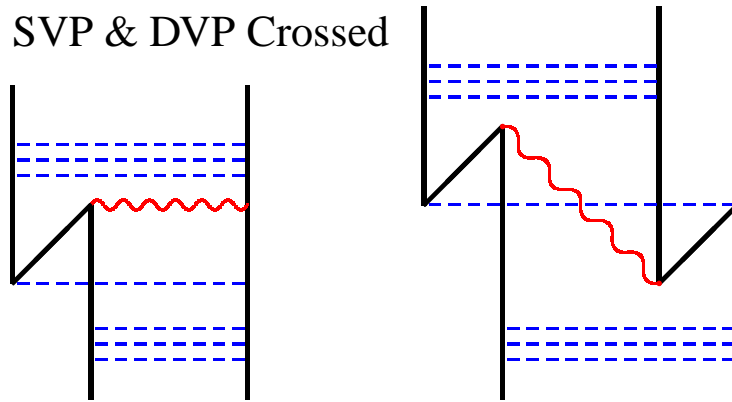
SVP & DVP



Cross Diagrams, VP

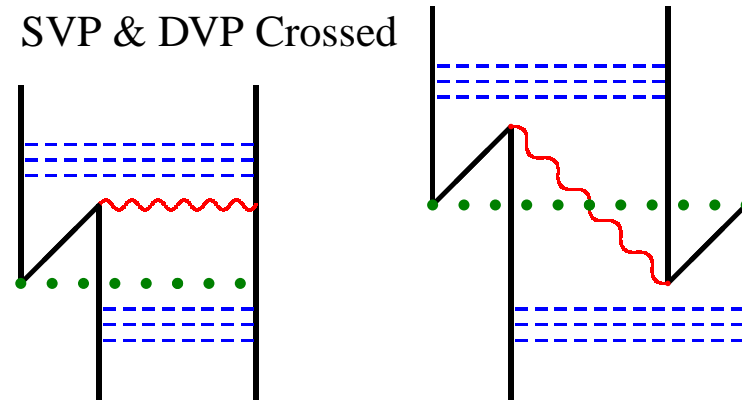
Coulomb - Breit

SVP & DVP Crossed



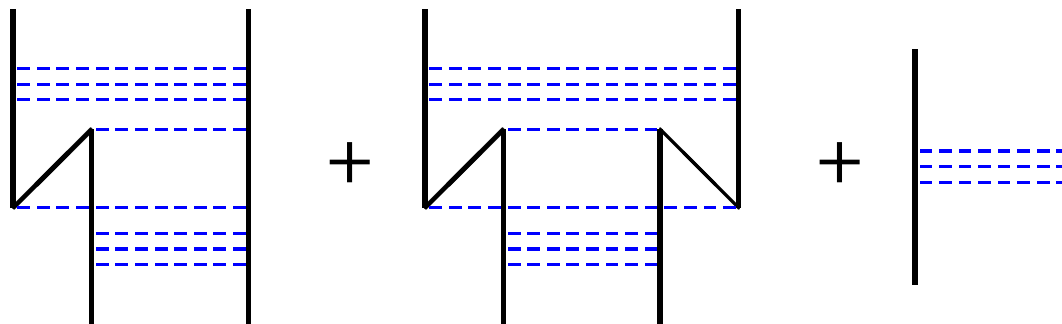
Breit - Breit

SVP & DVP Crossed

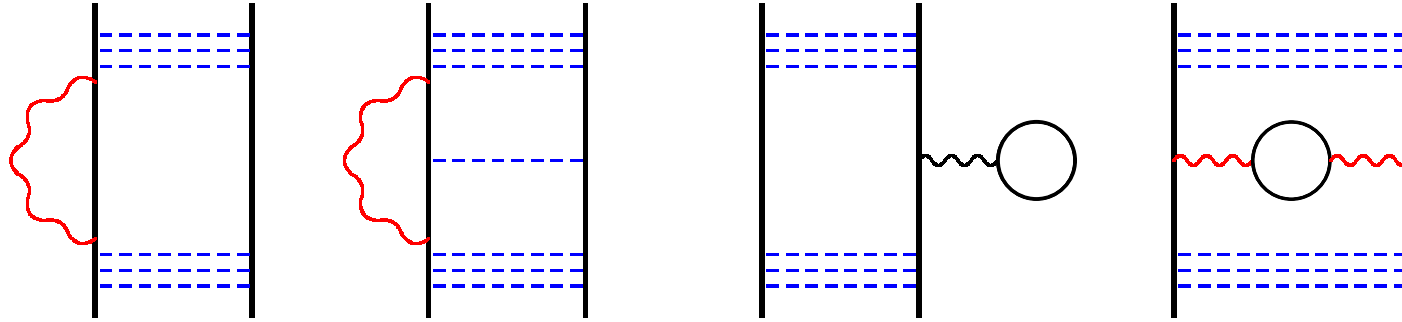


Coulomb - Coulomb

SVP & DVP

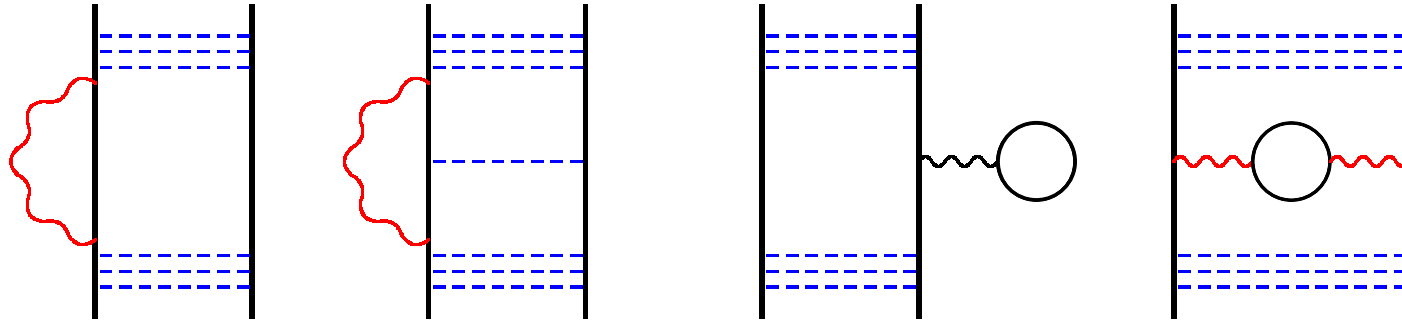


Radiative Effects

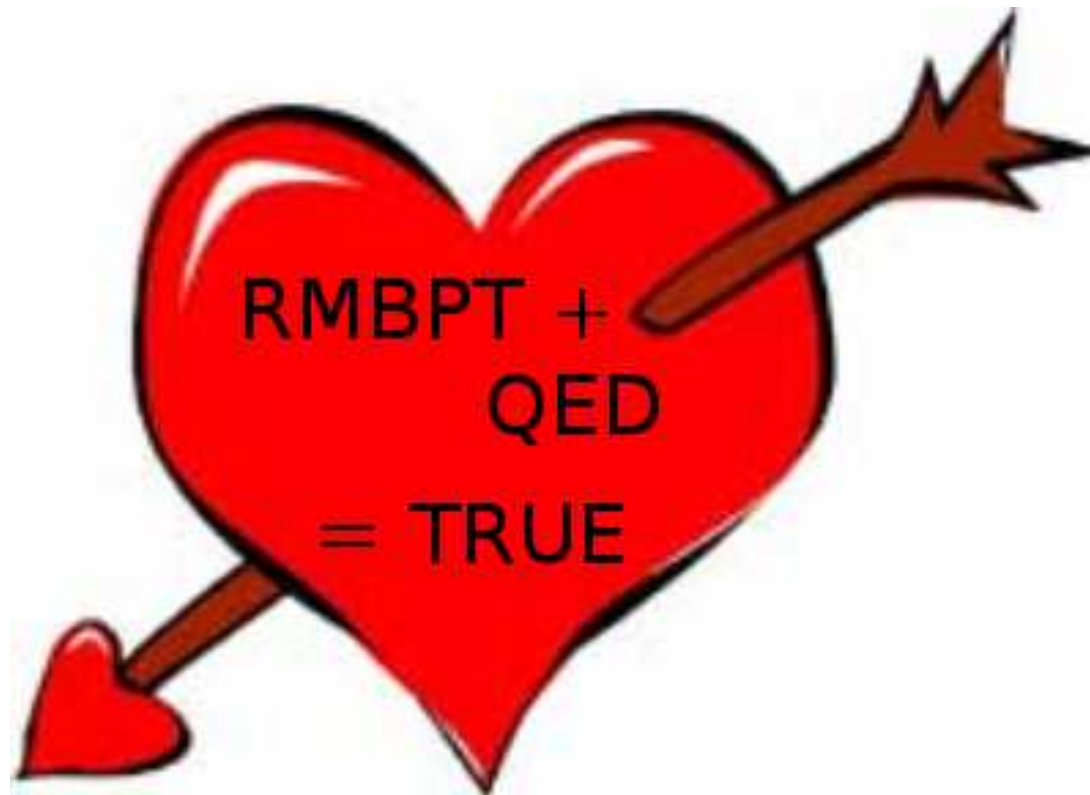


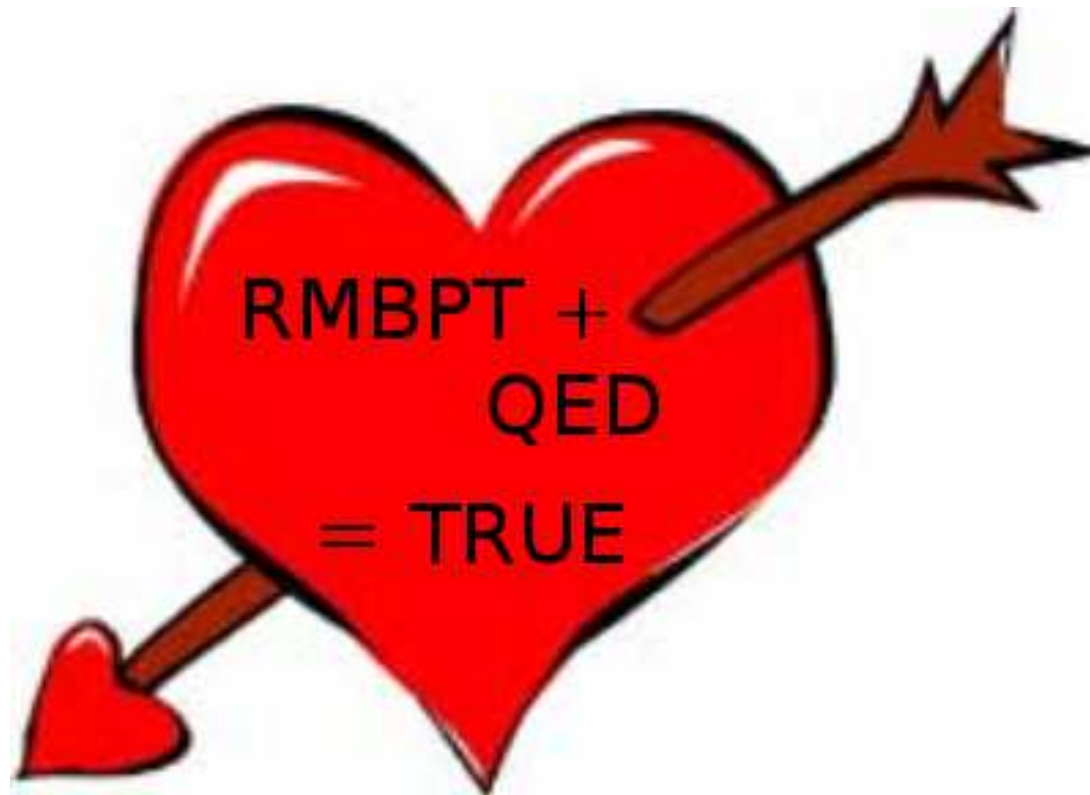
- Two approaches are under consideration
 - The Partial Wave Renormalization

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)





First happily married after a successful test of the radiative effects