Combined QED and Electron Correlation in He-like Systems

by

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Relativistic MBPT:

Breit interaction

$$H_B = -\frac{1}{2}\sum_{i<1}\left[\alpha_i \cdot \alpha_j + \frac{(\alpha_i \cdot r_{ij})(\alpha_j \cdot r_{ij})}{r_{ij}^2}\right]$$

Relativistic MBPT:

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Dirac-Coulomb-Breit Hamiltonian (NVPA)

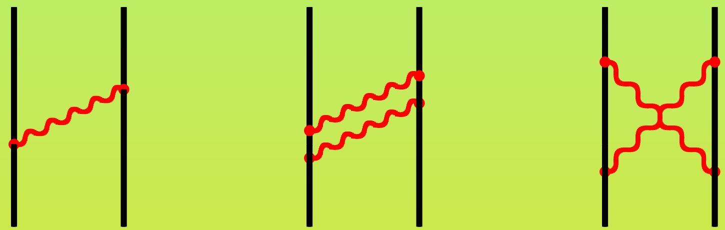
$$H = \Lambda_+\left[\sum_{i=1}^{N} h_D(i) + \sum_{i<j}^{N}\frac{1}{r_{ij}} + H_B\right]\Lambda_+$$

Not relativistically covariant

Effects beyond Dirac-Coulomb-Breit

referred to as QED effects

Non-radiative effects (retardation, virtual pairs)



Retarded Breit **Araki-Sucher**

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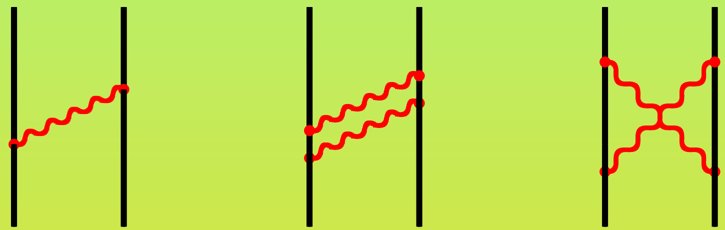

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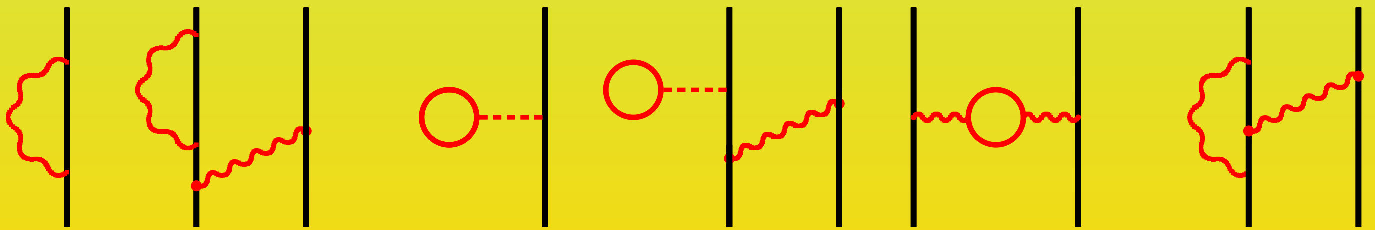
Radiative effects



Self energy **Vacuum polarization** **Vertex corr.**

- **ENERGY contributions due to QED can be evaluated by S-matrix or Green's function**
- **No information of wave function/operator**
- **In practice only two-photon exchange**
- **Poor treatment of electron correlation**

First relativistically covariant theory:

Bethe-Salpeter eqn

Salpeter and Bethe 1951; Gell-Mann and Low 1951

$$\Psi(E) = G_0(E)\,\Sigma(E)\,\Psi(E)$$

$$(E - H_0)\Psi(E) = \hat{\mathcal{V}}(E)\,\Psi(E)$$

Can QED be treated systematically within the framework of relativistic MBPT?

Covariant evolution operator

Evolution operator

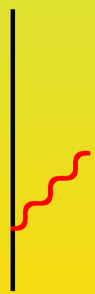
Interaction picture

$$|\Psi(t)\rangle = \hat{U}(t,t_0)\,|\Psi(t_0)\rangle$$

$$\hat{U}(t,t_0) = \sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n}{n!} \int_{t_0}^{t} \mathrm{d}x_1^4 \ldots \int_{t_0}^{t} \mathrm{d}x_n^4 \, T\Big[\hat{\mathcal{H}}'(x_1) \ldots \hat{\mathcal{H}}'(x_n)\Big]$$

$$\hat{\mathcal{H}}'(x) = -e\hat{\psi}^{\dagger}\alpha^{\mu} A_{\mu}\hat{\psi}$$

interaction with the electro-magnetic field



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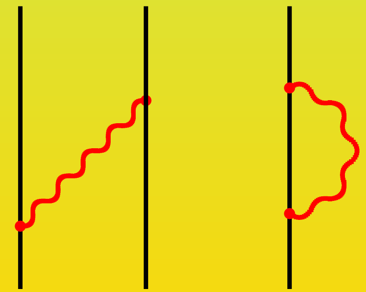
Two interactions exchange of virtual photon



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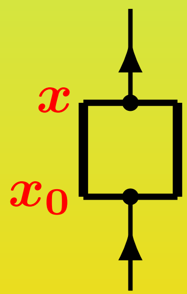


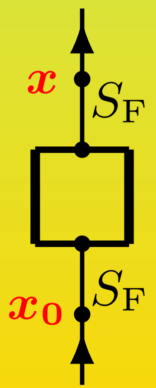
Relativistically non-covariant

Covariant evolution operator

Can be made be made covariant by inserting extra electron-field operators

$$\hat{U}_{\rm Cov}(t,t_0)=\sum_{n=0}^{\infty}\frac{(-\mathrm{i})^n}{n!}\int\cdots\int \mathrm{d}^4x_1\cdots\mathrm{d}^4x_n$$

$$\times T\big[\hat{\mathcal{H}}'(x_1)\cdots\hat{\mathcal{H}}'(x_n)\;\underbrace{\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}^\dagger(x_0)\hat{\psi}(x_0)}\big]$$



Relativistically covariant

Green's operator

Green's operator is the linked part of the covariant evolution operator

$$\hat{\mathcal{G}}(t,t_0) = \hat{U}_{\text{Cov}}(t,t_0)_{\text{linked}}$$

Green's operator

$$\hat{\mathcal{G}}(t,t_0) = \sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n}{n!} \left[\int \cdots \int \mathrm{d}^4x_1 \cdots \mathrm{d}^4x_n \right.$$

$$\left. \times T\left[\hat{\mathcal{H}}'(x_1)\cdots\hat{\mathcal{H}}'(x_n)\ \underbrace{\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}^\dagger(x_0)\hat{\psi}(x_0)}\right]\right]_{\text{LINKED}}$$

Green's operator

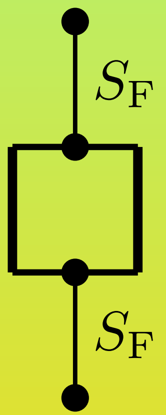
$$\hat{\mathcal{G}}(t,t_0) = \sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n}{n!} \Bigg[\int \cdots \int \mathrm{d}^4x_1 \cdots \mathrm{d}^4x_n \times T\Big[\hat{\mathcal{H}}'(x_1)\cdots\hat{\mathcal{H}}'(x_n)\, \underbrace{\hat{\psi}^\dagger(x)\hat{\psi}(x)\hat{\psi}^\dagger(x_0)\hat{\psi}(x_0)}\Big] \Bigg]_{\text{LINKED}}$$

Green's function

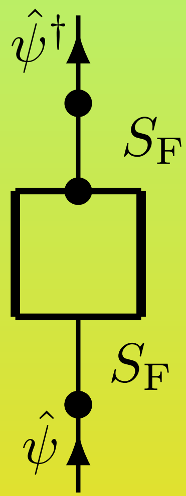
$$G(x,x_0) = \sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n}{n!} \Bigg[\int \cdots \int \mathrm{d}^4x_1 \cdots \mathrm{d}^4x_n \times \langle 0|T\Big[\hat{\mathcal{H}}'(x_1)\cdots\hat{\mathcal{H}}'(x_n)\, \underbrace{\hat{\psi}(x)\hat{\psi}^\dagger(x_0)}\Big] \Bigg]_{\text{LINKED}}$$

Green's operator

Green's FUNCTION



Green's OPERATOR



Green's operator unifies MBPT with QED

Open part repr. MBPT wave operator

$$\hat{\Omega} = 1 + \hat{\mathcal{G}}_{\mathrm{op}}(0)$$

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Open part repr. MBPT wave operator

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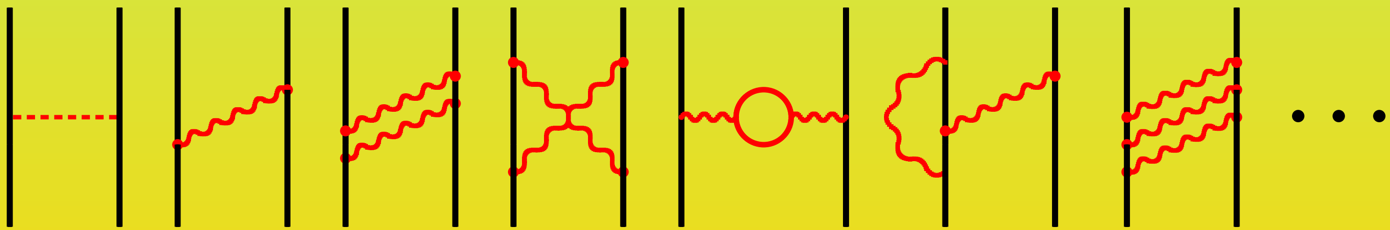
Handle energy-dependent interactions of QED

$\hat{\mathcal{V}}(E)$:



Perturbation expansion

First order: $\hat{\Omega}^{(1)} = \Gamma_Q \hat{\mathcal{V}}(E_0)$ $\quad \Gamma_Q = \frac{Q}{E_0 - H_0}$

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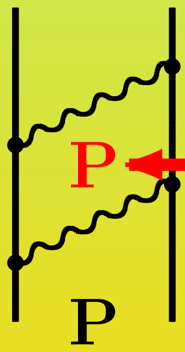
Second order:

$$\hat{\Omega}^{(2)} = \Gamma_Q \hat{\mathcal{V}}(E_0)\,\hat{\Omega}^{(1)} - \Gamma_Q\,\hat{\Omega}^{(1)}\hat{\mathcal{V}}_{\text{eff}}(E_0) + \Gamma_Q \left(\frac{\partial \hat{\mathcal{V}}}{\partial \mathcal{E}}\right)_{E_0} \hat{\mathcal{V}}_{\text{eff}}(E_0)$$

$\hat{\mathcal{V}}_{\text{eff}} = P\hat{\mathcal{V}}\hat{\Omega}P$

"folded" "reference-state contribution"

model-space-state contributions



Finite residuals after eliminating (quasi)-singularities due to intermediate model-space state

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All orders:

$$\hat{\Omega} = \Gamma_Q \hat{\mathcal{V}}(E)\,\hat{\Omega} - \Gamma_Q\,\hat{\Omega}\,\hat{\mathcal{V}}_{\text{eff}}(E)$$

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All orders:

$$\hat{\Omega} = \Gamma_Q \hat{\mathcal{V}}(E)\,\hat{\Omega} - \Gamma_Q\,\hat{\Omega}\,\hat{\mathcal{V}}_{\text{eff}}(E)$$

$$(E_0 - H_0)\hat{\Omega} = \hat{\mathcal{V}}(E)\,\hat{\Omega} - \hat{\Omega}\hat{\mathcal{V}}_{\text{eff}}(E)$$

Bethe-Salpeter-Bloch equation

Perturbation expansion

First order: $\hat{\Omega}^{(1)} = \Gamma_Q \hat{\mathcal{V}}(E_0)$ $\quad \Gamma_Q = \frac{Q}{E_0 - H_0}$

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All orders:

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$$(E - H_0)\Psi = \hat{\mathcal{V}}(E)\,\Psi$$

Bethe-Salpeter equation

Implementation

Difficult to evaluate the energy derivative

$$\hat{\Omega}^{(2)} = \Gamma_Q \hat{\mathcal{V}}(E_0)\,\hat{\Omega}^{(1)} - \Gamma_Q\,\hat{\Omega}^{(1)} V_{\mathrm{eff}} + \Gamma_Q \left(\frac{\partial \hat{\mathcal{V}}}{\partial \mathcal{E}}\right)_{E_0} \hat{\mathcal{V}}_{\mathrm{eff}}$$

Simpler in

Extended Fock space

Implementation

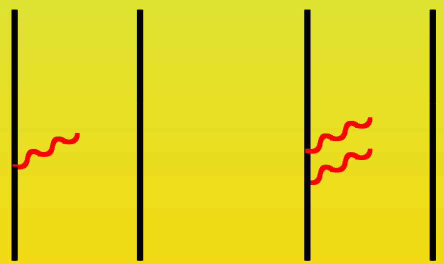
Difficult to evaluate the energy derivative

$$\hat{\Omega}^{(2)} = \Gamma_Q \hat{\mathcal{V}}(E_0)\,\hat{\Omega}^{(1)} - \Gamma_Q\,\hat{\Omega}^{(1)} V_{\text{eff}} + \Gamma_Q \left(\frac{\partial \hat{\mathcal{V}}}{\partial \mathcal{E}}\right)_{E_0} \hat{\mathcal{V}}_{\text{eff}}$$

Simpler in

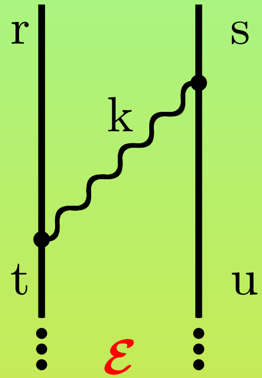
Extended Fock space

Uncontracted perturbations $\hat{\mathcal{H}}'(x) = -\hat{\psi}^\dagger \alpha^\mu A_\mu \hat{\psi}$
go outside the Hilbert space with constant n:o photons



Implementation

Single-photon exchange. Coulomb gauge



$$V_{sp}(\mathcal{E}) = \frac{1}{r_{12}} + \int_0^\infty \frac{f_C(k)\,\mathrm{d}k}{\mathcal{E}-\varepsilon_r-\varepsilon_u \mp (k-\mathrm{i}\eta)}$$

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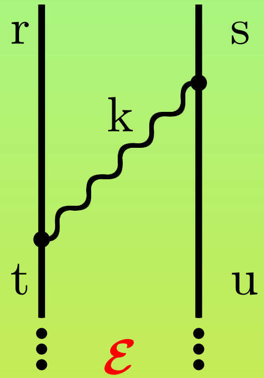


$$V_{sp}(\mathcal{E}) = \frac{1}{r_{12}} + \int_0^\infty \frac{f_C(k)\,\mathrm{d}k}{\mathcal{E}-\varepsilon_r-\varepsilon_u \mp (k - \mathrm{i}\eta)}$$

$$f_C(k) = \boldsymbol{\alpha_1}\cdot\boldsymbol{\alpha_2}\,\frac{\sin(kr_{12})}{\pi r_{12}} - (\boldsymbol{\alpha_1}\cdot\boldsymbol{\nabla_1})\,(\boldsymbol{\alpha_2}\cdot\boldsymbol{\nabla_2})\,\frac{\sin(kr_{12})}{\pi k^2\, r_{12}}$$

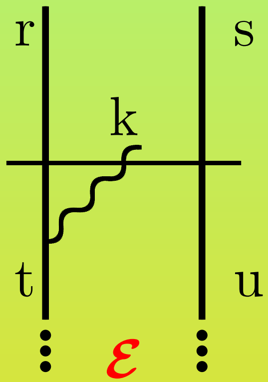
$$V_{sp}(\mathcal{E}) = \frac{1}{r_{12}} + \frac{V^l(kr_1)\cdot V^l(kr_2)}{\mathcal{E}-\varepsilon_r-\varepsilon_u \mp (k - \mathrm{i}\eta)} +$$

Implementation

Fock-space Bloch eqn:

$$(\hat{H}_0 - E_0)P = (H'\hat{\Omega} - \hat{\Omega}\,V_{\mathrm{eff}})P$$

$$H' = 1/r_{12} + V^l(kr_1) + V^l(kr_2)$$



$$\frac{V^l(kr_1)}{\mathcal{E} - \varepsilon_r - \varepsilon_u \mp (k - \mathrm{i}\eta)}$$

Implementation

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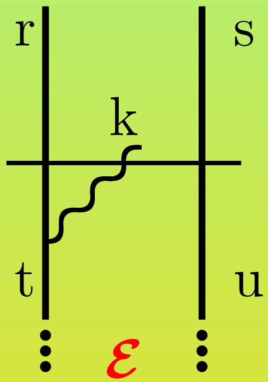

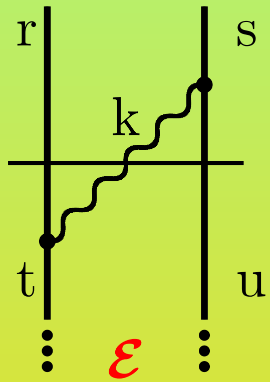

$$\frac{V^l(kr_1)}{\mathcal{E}-\varepsilon_r-\varepsilon_u\mp(k-\mathrm{i}\eta)} \qquad \frac{V^l(kr_1)\cdot V^l(kr_2)}{\mathcal{E}-\varepsilon_r-\varepsilon_u\mp(k-\mathrm{i}\eta)}$$

Extra denominator in Fock space yields energy dependence

$$V_{sp}(\mathcal{E}) = \frac{1}{r_{12}} + \frac{V^l(kr_1)\cdot V^l(kr_2)}{\mathcal{E}-\varepsilon_r-\varepsilon_u\mp(k-\mathrm{i}\eta)} + \qquad V^l(kr) \propto j_l(kr)\boldsymbol{\alpha}\boldsymbol{C}^l$$

Perturbation energy independent

Implementation

Fock-space Bloch eqn:

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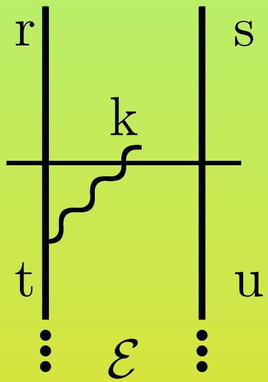
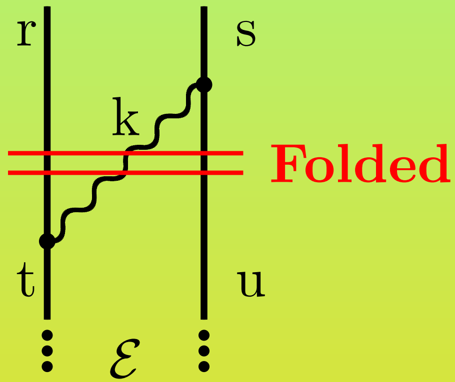




$$\frac{V^l(kr_1)}{\mathcal{E}-\varepsilon_r-\varepsilon_u\mp(k-\mathrm{i}\eta)} \qquad -\frac{V^l(kr_1)\cdot V^l(kr_2)}{(\mathcal{E}-\varepsilon_r-\varepsilon_u\mp(k-\mathrm{i}\eta))^2}$$

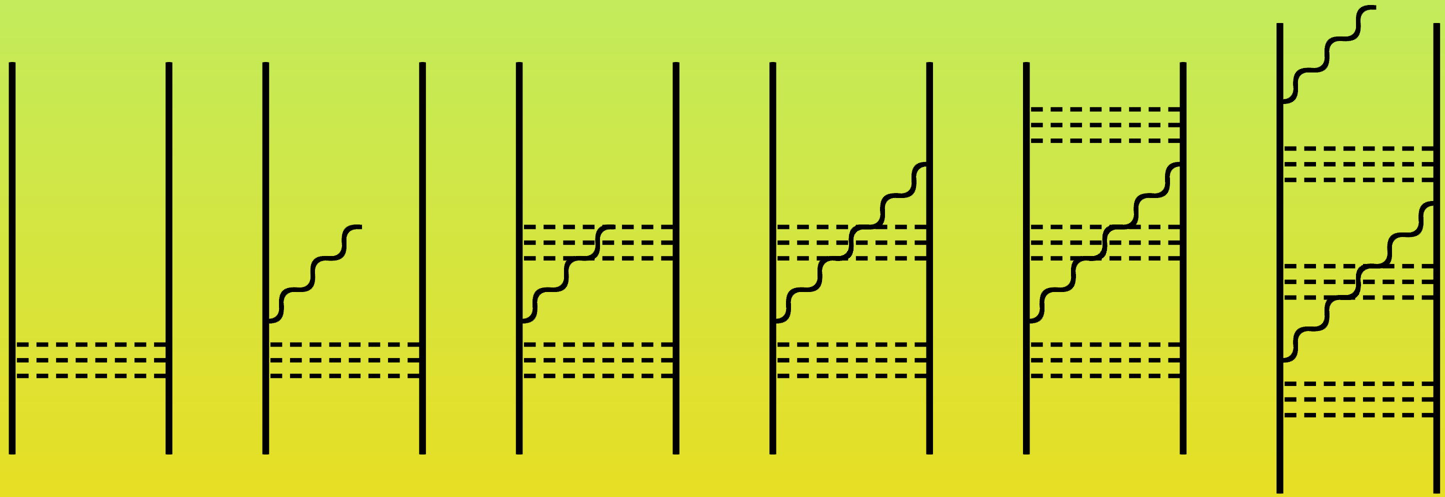
Extra denominator in Fock space yields energy dependence

Extra folded diagram in Fock space yields energy derivative

Implementation

$$(\hat{H}_0 - E_0)P = (H'\hat{\Omega} - \hat{\Omega}\, V_{\text{eff}})P$$

$$H' = 1/r_{12} + V^l(kr_1) + V^l(kr_2)$$



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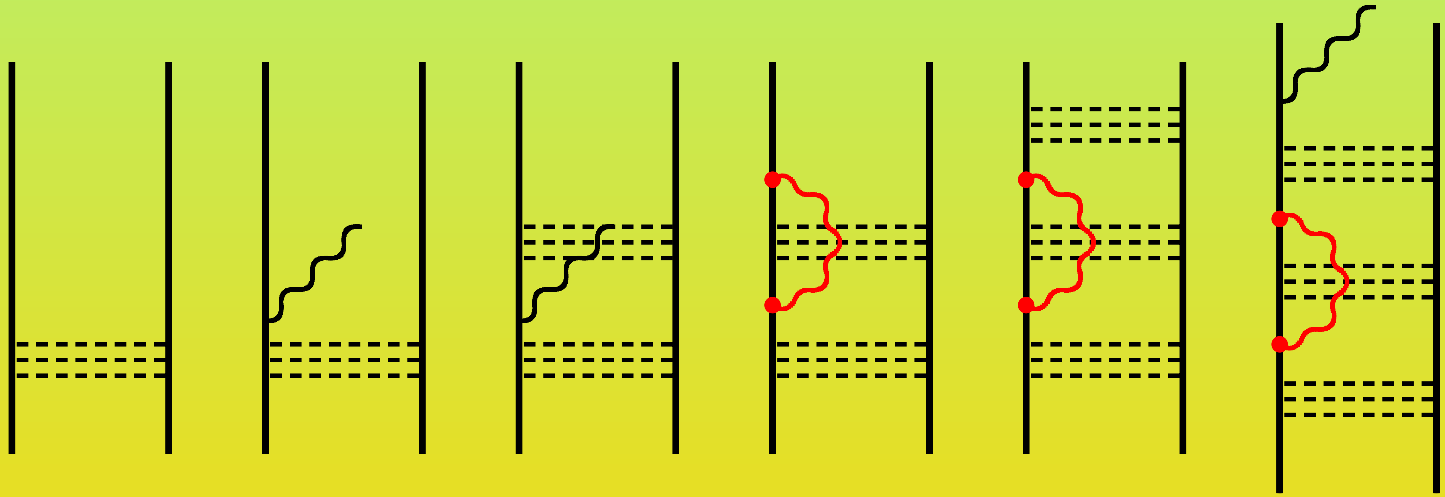

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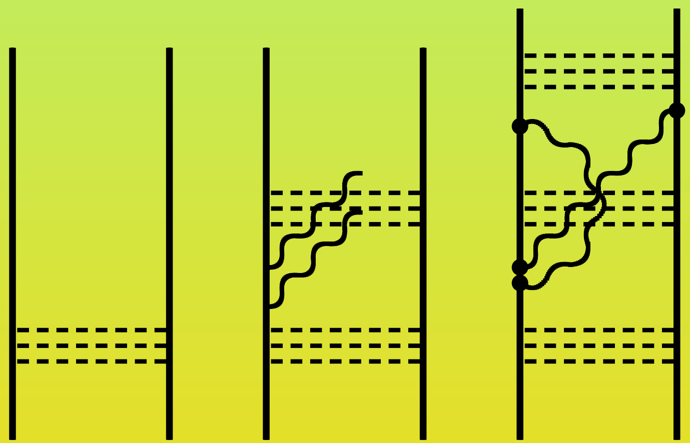
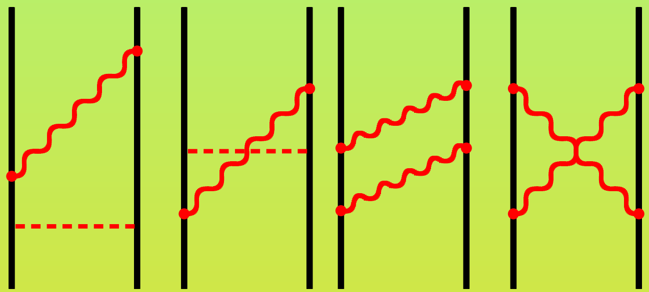


Presently not feasible

Heliumlike neon ground state

Non-radiative QED effects

beyond Dirac-Coulomb-Breit (in μH)



239 **-117** **3** **10**

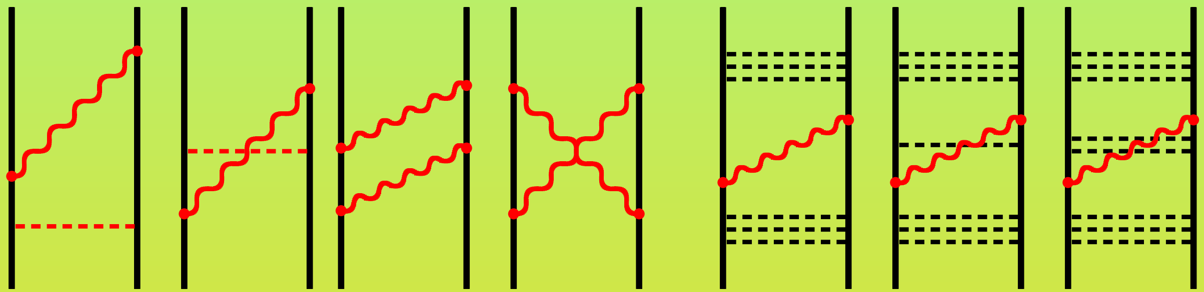
135

Two photons

Heliumlike neon ground state

Non-radiative QED effects

beyond Dirac-Coulomb-Breit (in μH)



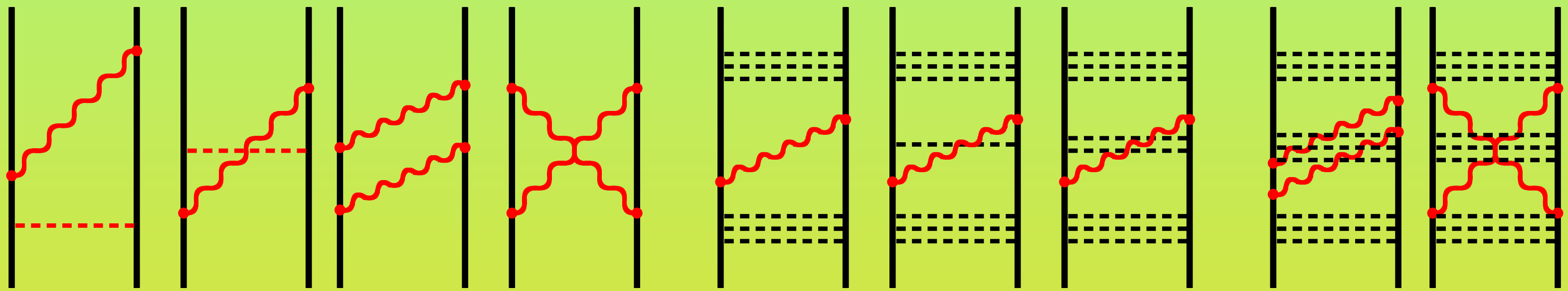
239	-117	3	10	-95	44	1

135 — Two photons

-51 — Single retarded photon with h-o correlation

Heliumlike neon ground state

Non-radiative QED effects
beyond Dirac-Coulomb-Breit (in μH)



239 | -117 | 3 | 10 | -95 | 44 | 1

135 — Two photons

-51 — Single retarded photon with h-o correlation

(1-3) — Remaining effects

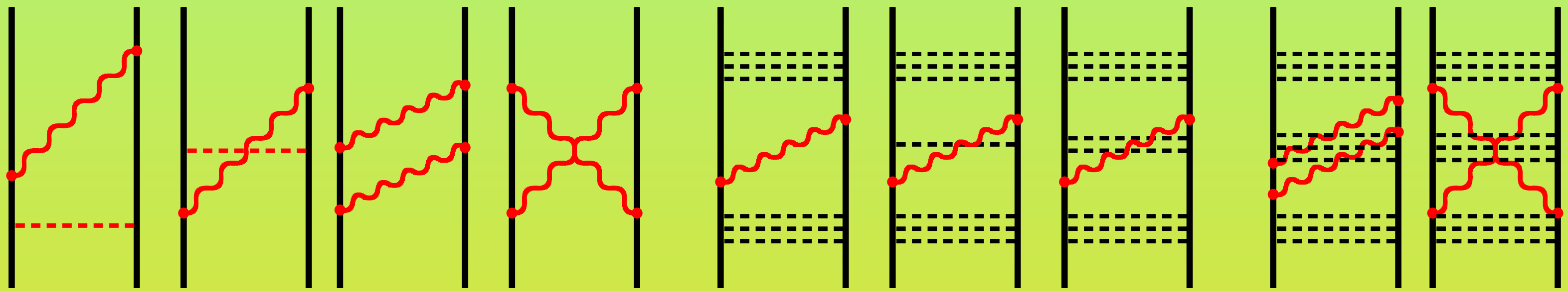
Combined QED-Correlation effects beyond two-photon exchange

Numerical results

Heliumlike neon ground state

Non-radiative QED effects

beyond Dirac-Coulomb-Breit (in μH)



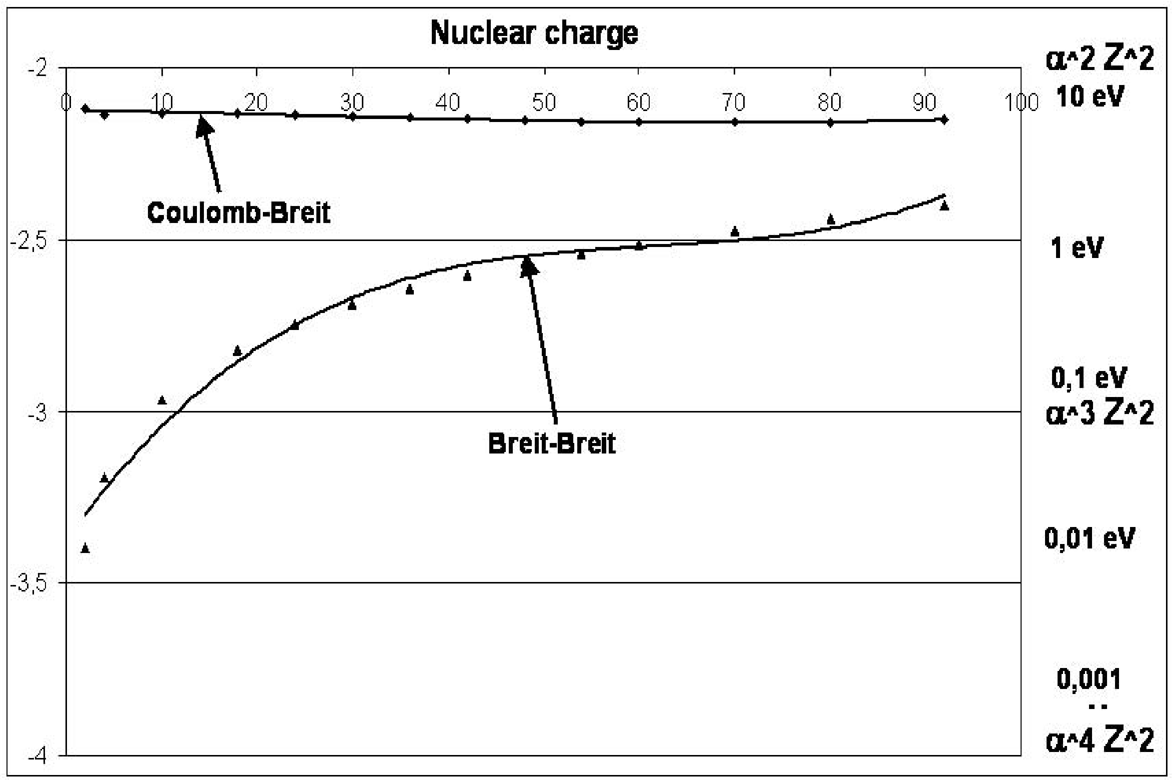
239 | **-117** | **3** | **10** → **135** Two photons

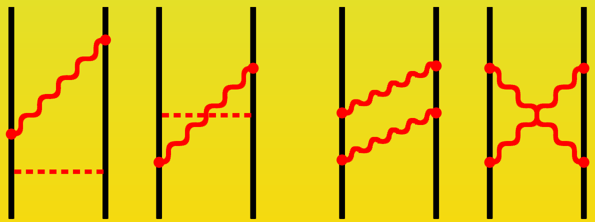
-95 | **44** | **1** → **-51** Single retarded photon with h-o correlation

(1-3) Remaining effects

Most of the remaining effect due to single retarded and one or more instantaneous Breit interactions which can also be evaluated

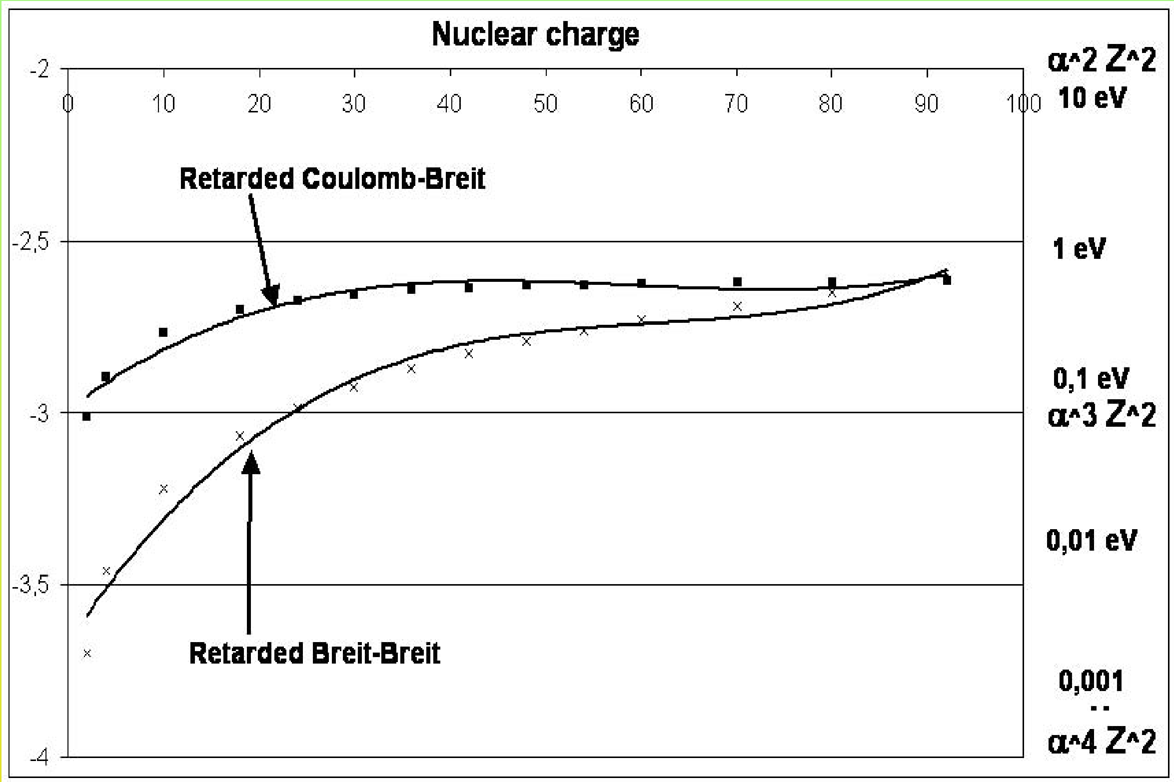
Breit interaction (unretard. and retard.) for He-like ions

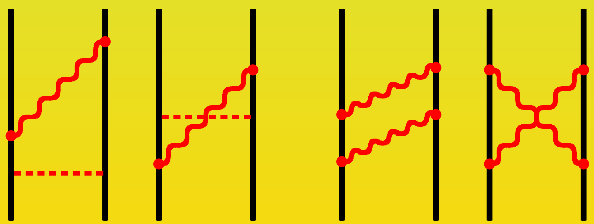




Coul-Breit Breit-Breit

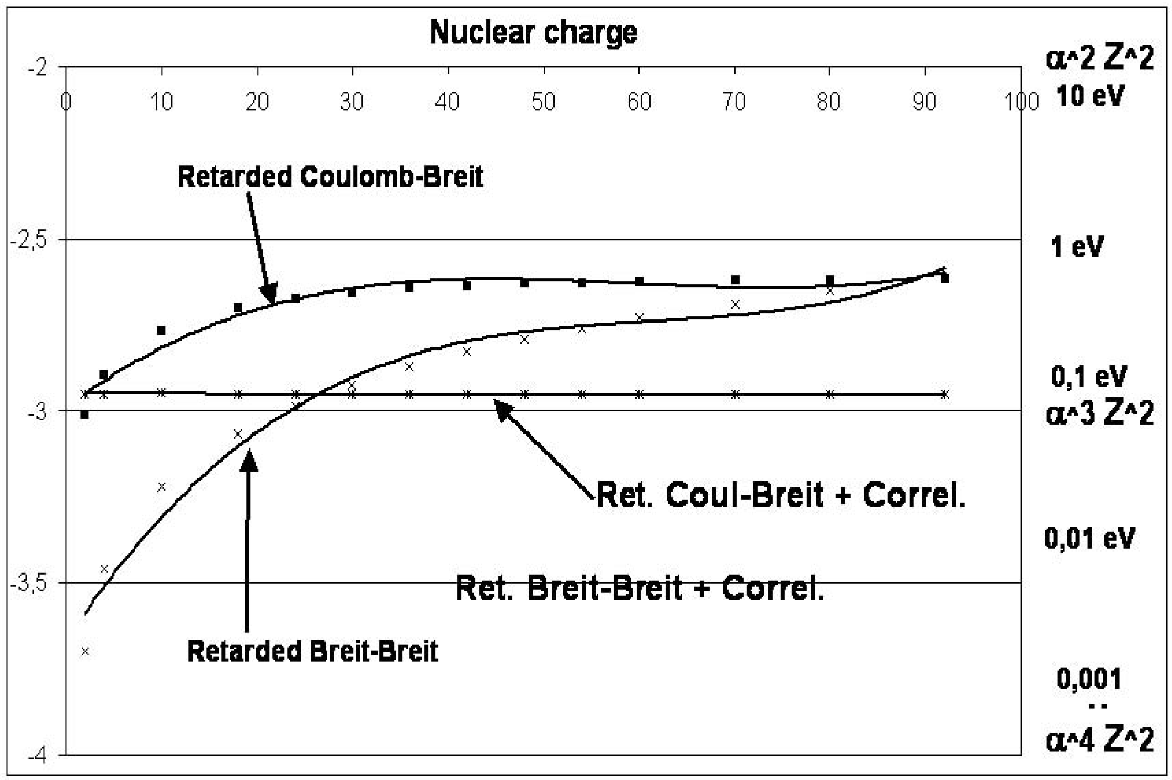
Retarded Breit interaction for He-like ions

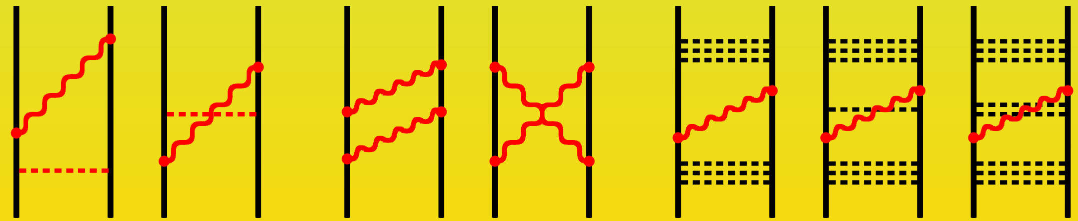




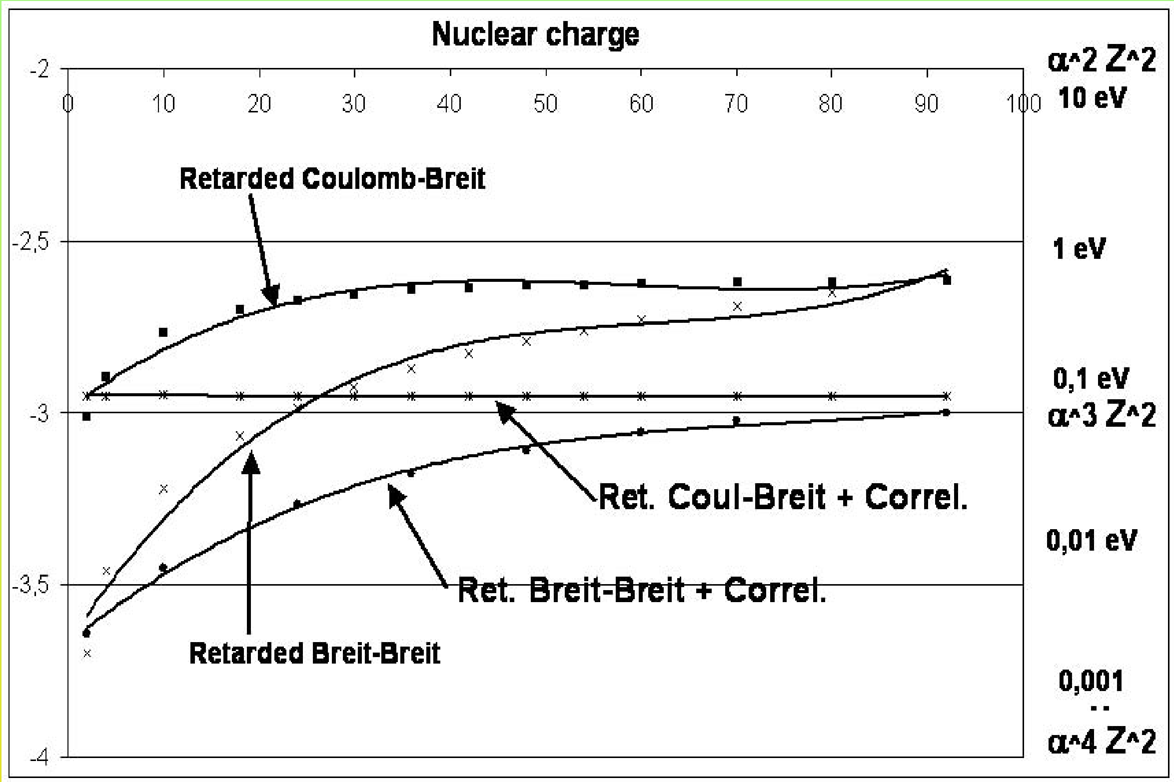
Coul-Breit Breit-Breit

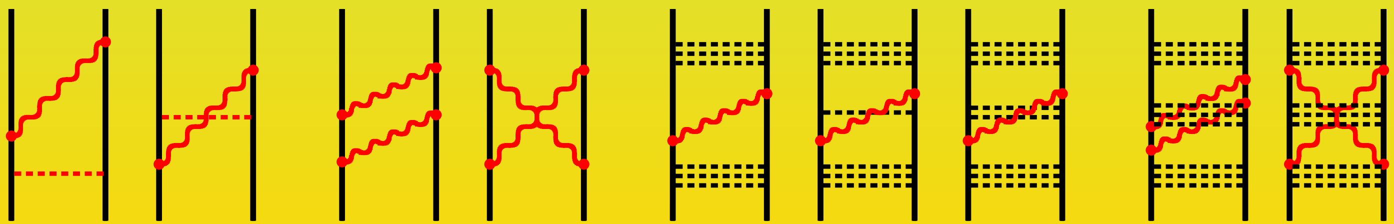
Retarded Breit interaction for He-like ions





Retarded Breit interaction for He-like ions

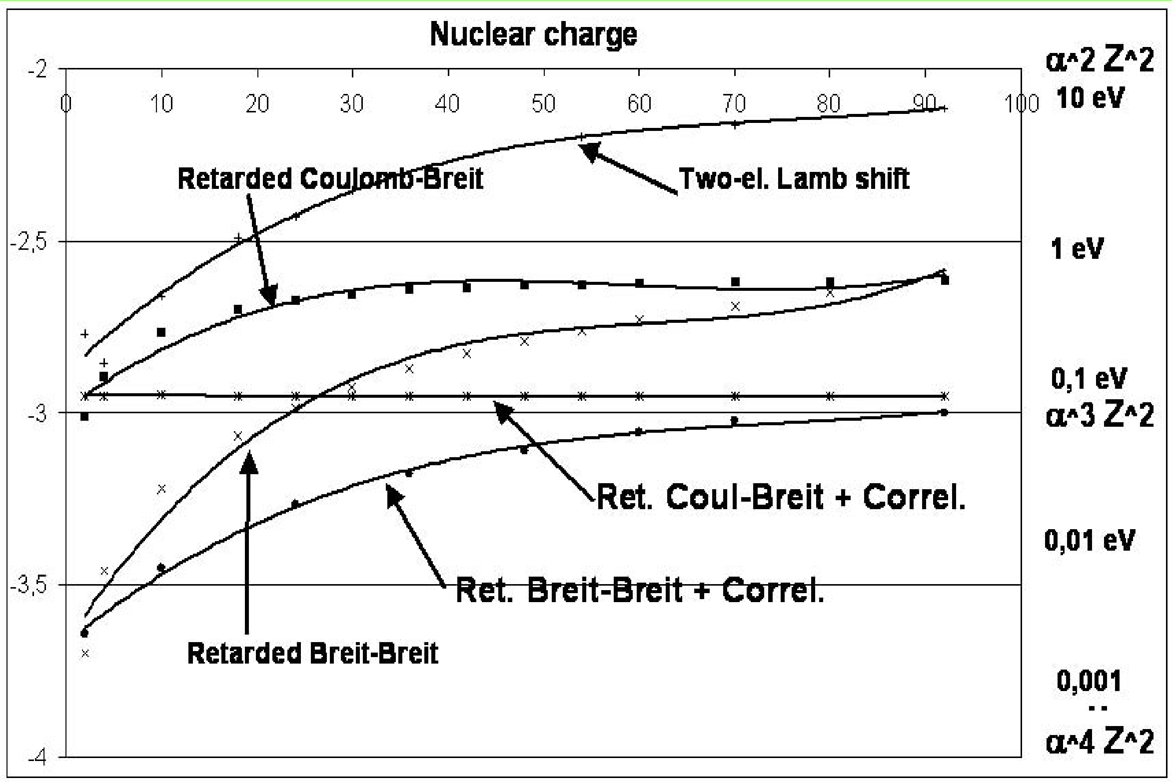


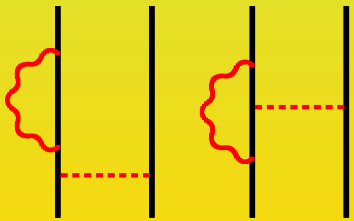


Coul-Breit Breit-Breit Coul-Breit + correl. Breit-Breit + correl.

Numerical results

QED effects for He-like ions





Two-el. Lamb shift

Conclusions

- **QED with high-order electron correlation can be evaluated numerically by means of Covariant-Evolution-Operator/ Green's-Operator technique**

Conclusions

- **QED with high-order electron correlation can be evaluated numerically by means of Covariant-Evolution-Operator/ Green's-Operator technique**

- **In going beyond first-order QED corrections, combined QED-correlation important for light and medium-heavy ions**

Publications

Recent publications

- **I.Lindgren, S.Salomonson, and B.Åsén**
  Physics Reports, 389, 161 (2004)
- **I.Lindgren, S.Salomonson and D.Hedendahl**
  Can. J. Phys. 83, 183 (2005)
  "Einstein Centennial paper"
- **I.Lindgren, S.Salomonson and D.Hedendahl**
  Phys. Rev. A73, 062502 (2006)