A Covariant Form of Relativistic Many-Body Calculations

Combining Many-Body and QED Effects

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Coworkers

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Introduction

Performing relativistic calculations covariantly implies that many-body effects (electron correl.) and quantum-electro-dynamical effects (QED) are treated simultaneously in a rigorous way

Why is that of interest?

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Heavy-ion research

Test of Quantum-Electro-Dynamics at strong fields

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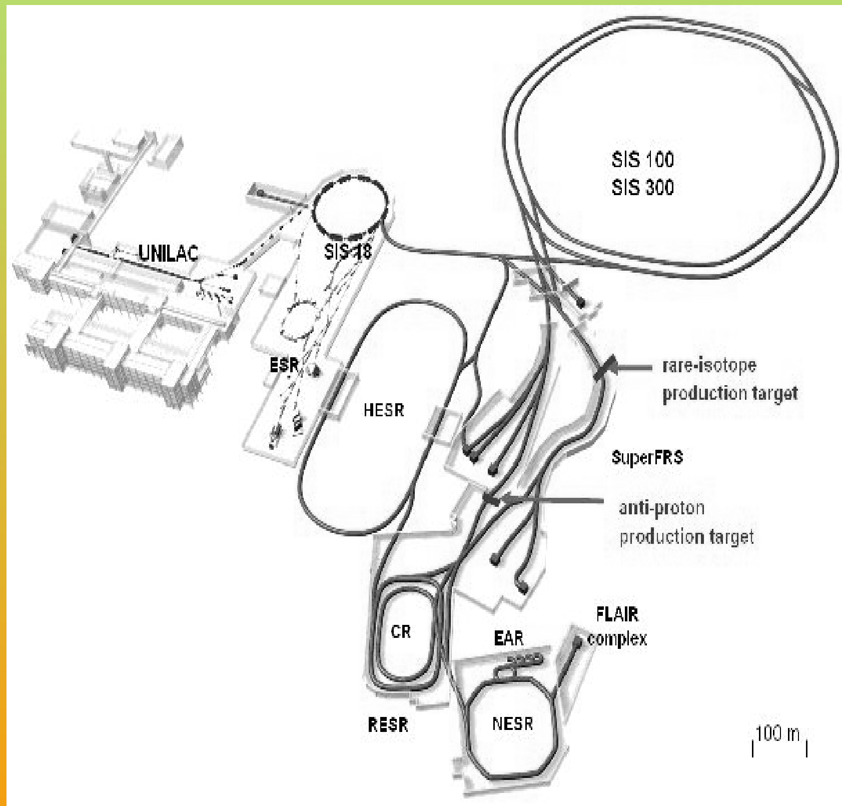
Heavy-ion research

Test of Quantum-Electro-Dynamics
at strong fields

Precision experiments on light systems

Can lead to independent determination of
fine-structure constant α

FAIR – **Facility for Antiproton and Ion Research**



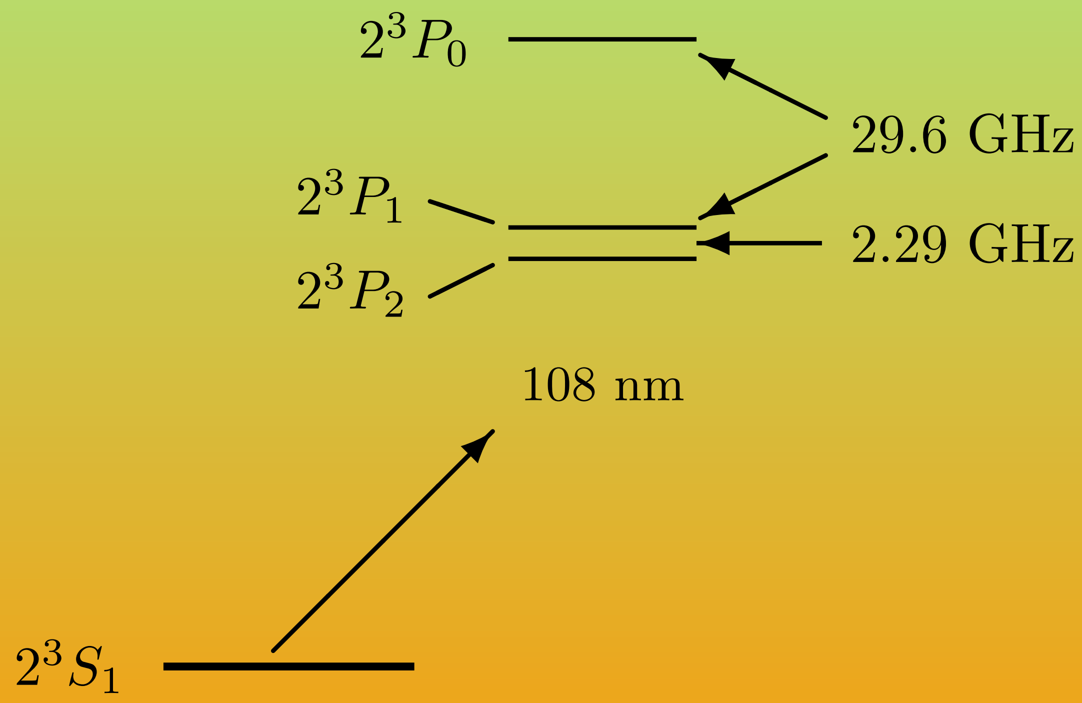
Introduction

Exciting new possibilities for heavy-ion research

New situation for theory

Requires further development of theory in order to match the new experimental situation

Fine structure of the helium atom

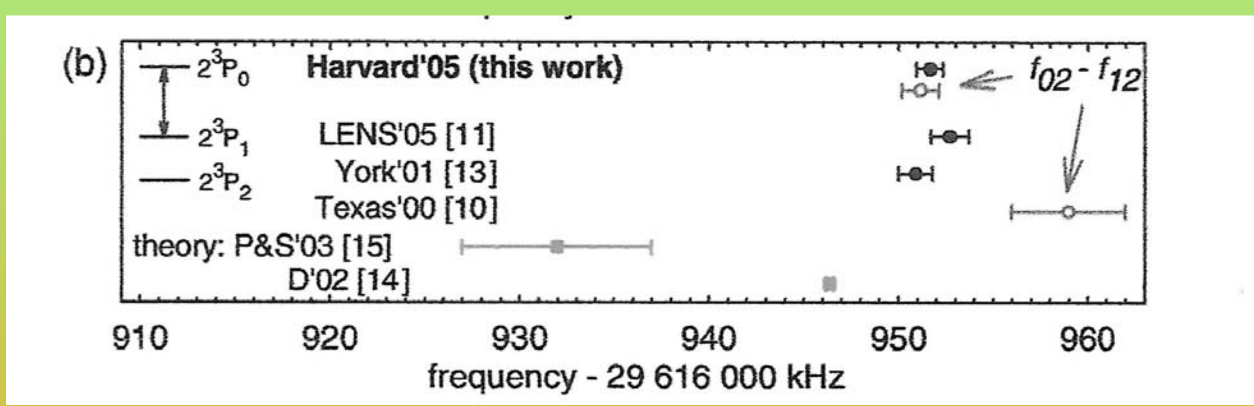


Fine structure of helium atom

Comparison between experimental and theoretical

fine structure for the $2\,^3P$ state of neutral helium

$^3P_0 - ^3P_1$



Exptl: Gabrielse, Inguscio...
Theory: Drake, Pachucki-Sapirstein

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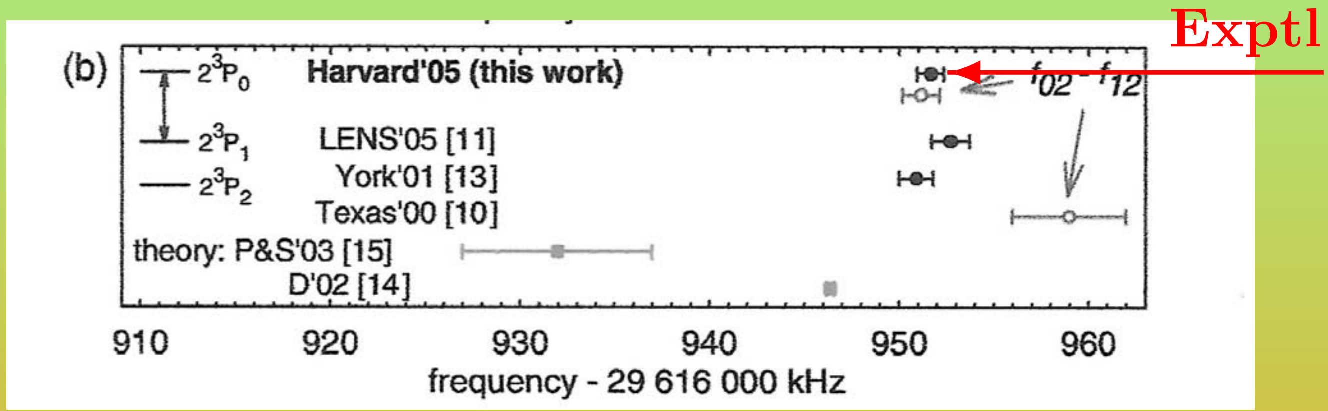

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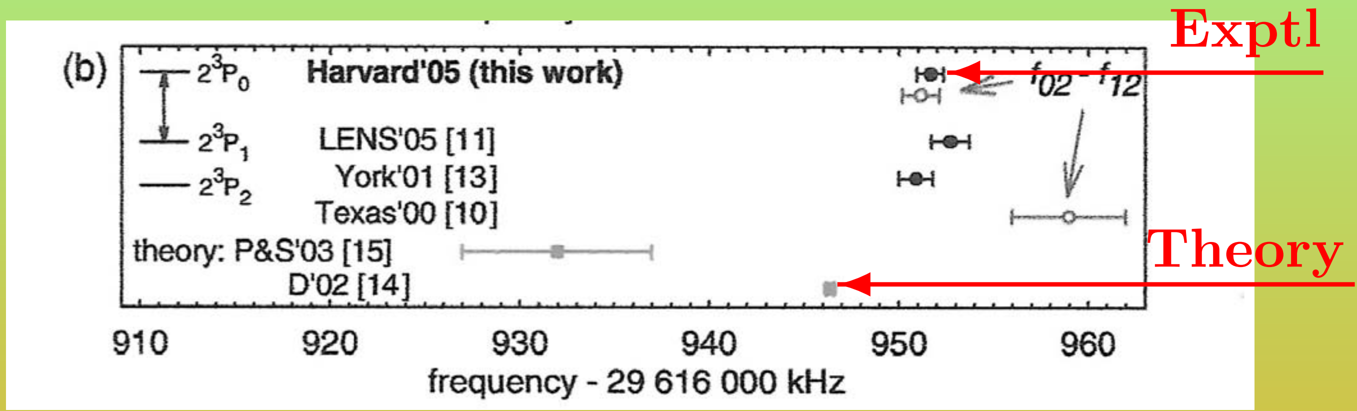

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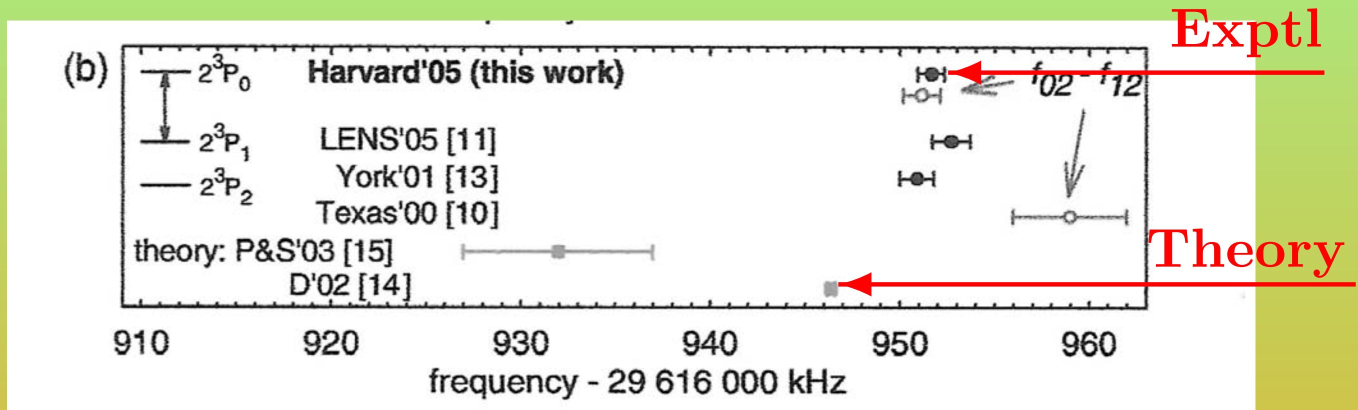
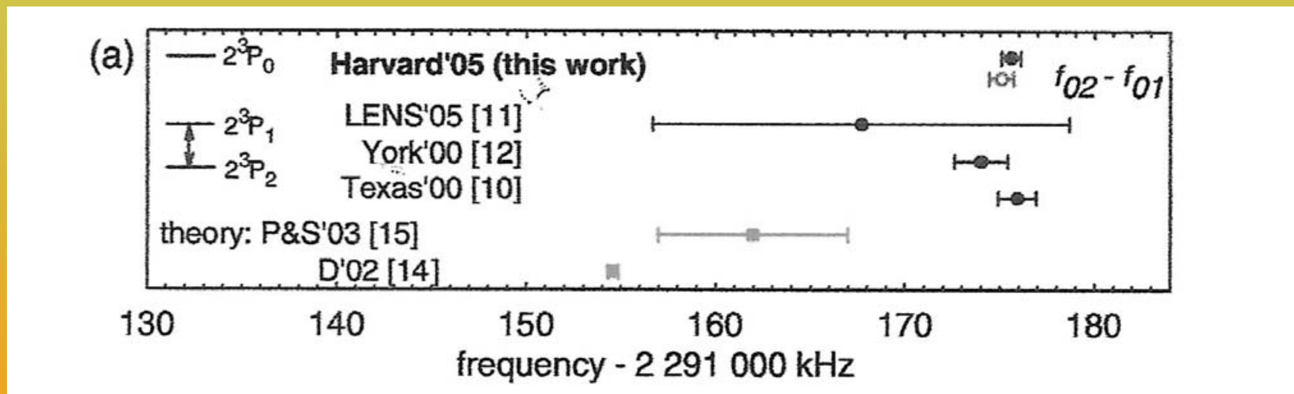


$^3P_1 - {}^3P_2$



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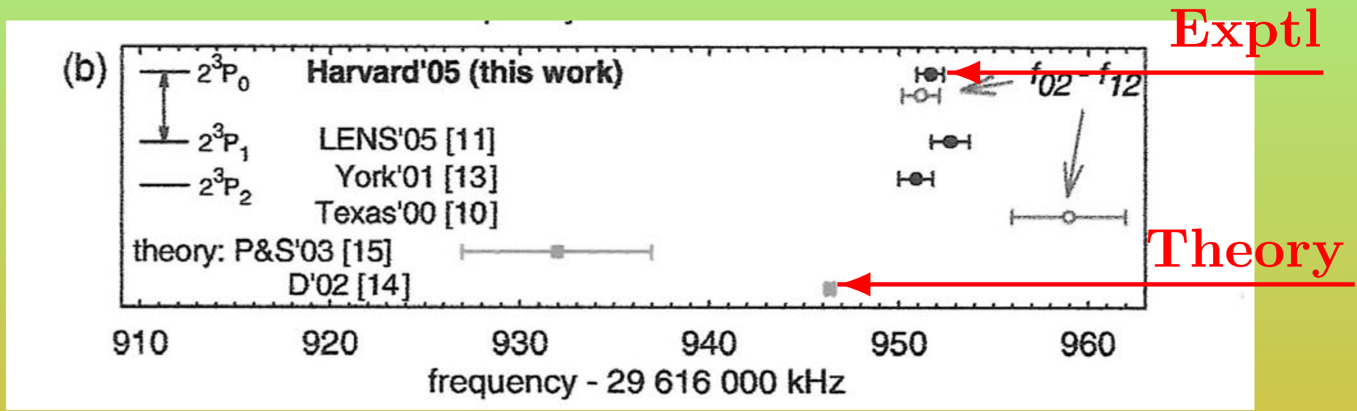

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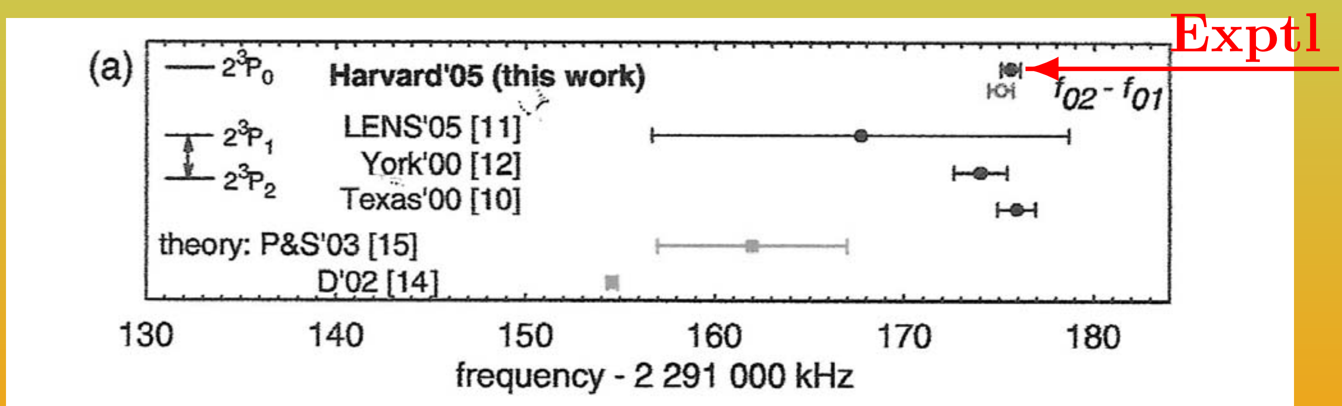

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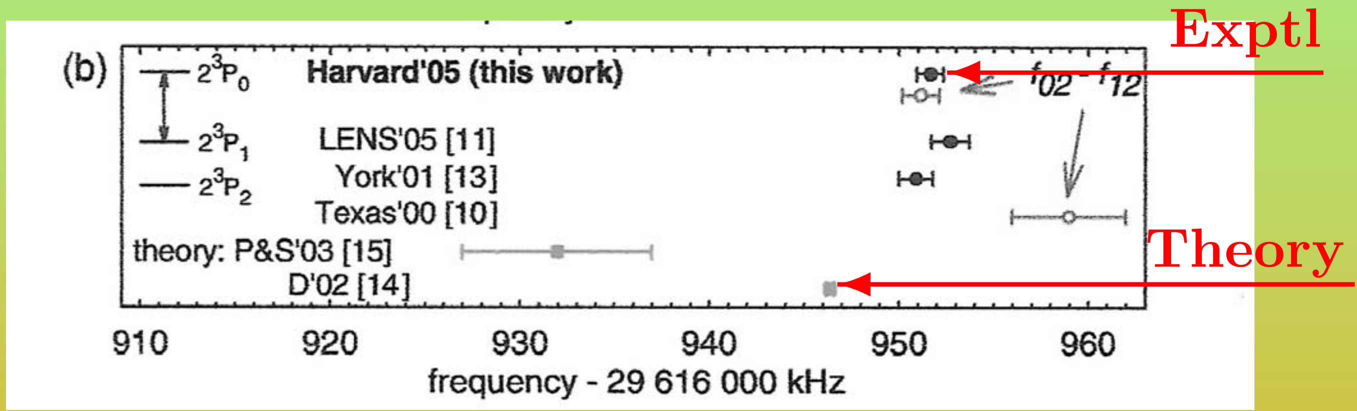

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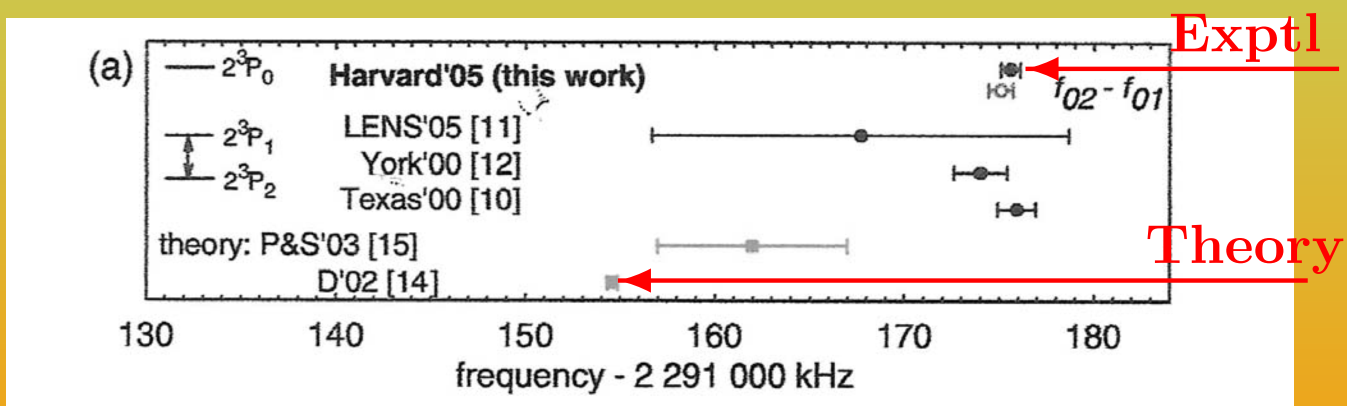

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Fine structure of helium atom

Once the theoretical discrepancies are resolved, this can lead to an independent

determination of the fine- structure constant α

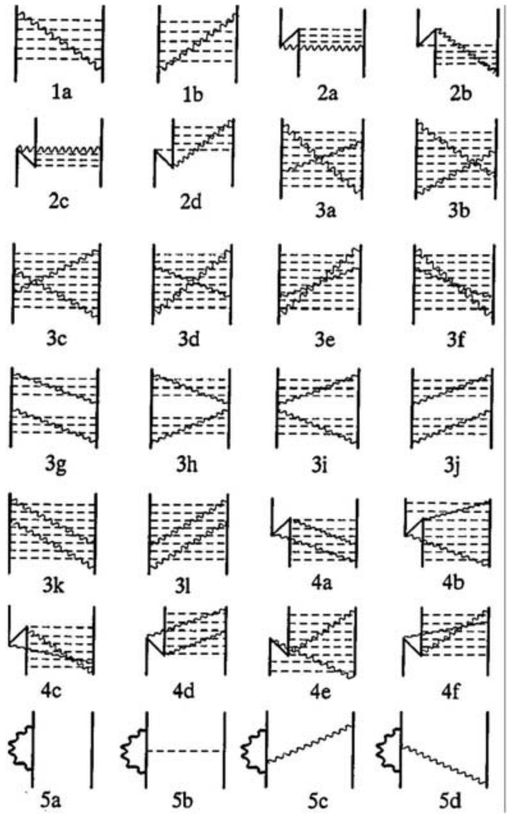
Analytical approach

Drake's calculations based upon non-relativistic Hylleraas-type wave functions

and analytical power expansion of relativistic and QED effects up to order $\alpha^7 mc^2$

Analytical approach

Drake, Zhang 1996



Analytical approach

One of 18 energy contributions

$$
\begin{aligned}
\Delta E_c^{(6)} = {} & \frac{ZZ_1\alpha}{2\pi^2}\frac{1}{32m_1^4}\int \frac{d\mathbf{k}_1}{k_1^2}\langle \phi_0(\mathbf{p}_1,\mathbf{p}_2)|\tfrac{1}{2}p_1^2|\mathbf{p}_1-\mathbf{k}_1|^2+\tfrac{11}{4}(p_1^4+|\mathbf{p}_1-\mathbf{k}_1|^2)-3[p_1^2+|\mathbf{p}_1-\mathbf{k}_1|^2] \\
& \times[p_1^2-\mathbf{p}_1\cdot\mathbf{k}_1-i\boldsymbol{\sigma}_1\cdot(\mathbf{p}_1\times\mathbf{k}_1)]|\phi_0(\mathbf{p}_1-\mathbf{k}_1,\mathbf{p}_2)\rangle+\frac{ZZ_2\alpha}{2\pi^2}\frac{1}{32m_2^4}\int\frac{d\mathbf{k}_2}{k_2^2}\langle\phi_0(\mathbf{p}_1,\mathbf{p}_2)|\tfrac{1}{2}p_2^2|\mathbf{p}_2+\mathbf{k}_2|^2 \\
& +\tfrac{11}{4}(p_2^4+|\mathbf{p}_2+\mathbf{k}_2|^2)-3[p_2^2+|\mathbf{p}_2+\mathbf{k}_2|^2][p_2^2+\mathbf{p}_2\cdot\mathbf{k}_2+i\boldsymbol{\sigma}_2\cdot(\mathbf{p}_2\times\mathbf{k}_2)]|\phi_0(\mathbf{p}_1,\mathbf{p}_2+\mathbf{k}_2)\rangle \\
& +\frac{Z_1Z_2\alpha}{2\pi^2}\frac{1}{32m_1^4}\int\frac{d\mathbf{k}}{k^2}\langle\phi_0(\mathbf{p}_1,\mathbf{p}_2)|\tfrac{1}{2}p_1^2|\mathbf{p}_1-\mathbf{k}|^2+\tfrac{11}{4}(p_1^4+|\mathbf{p}_1-\mathbf{k}|^4)-3[p_1^2+|\mathbf{p}_1-\mathbf{k}|^2] \\
& \times[p_1^2-\mathbf{p}_1\cdot\mathbf{k}-i\boldsymbol{\sigma}_1\cdot(\mathbf{p}_1\times\mathbf{k})]|\phi_0(\mathbf{p}_1-\mathbf{k},\mathbf{p}_2+\mathbf{k})\rangle+\frac{Z_1Z_2\alpha}{2\pi^2}\frac{1}{32m_2^4}\int\frac{d\mathbf{k}}{k^2}\langle\phi_0(\mathbf{p}_1,\mathbf{p}_2)|\tfrac{1}{2}p_2^2|\mathbf{p}_2+\mathbf{k}|^2 \\
& +\tfrac{11}{4}(p_2^4+|\mathbf{p}_2+\mathbf{k}|^4)-3[p_2^2+|\mathbf{p}_2+\mathbf{k}|^2][p_2^2+\mathbf{p}_2\cdot\mathbf{k}+i\boldsymbol{\sigma}_2\cdot(\mathbf{p}_2\times\mathbf{k})]|\phi_0(\mathbf{p}_1-\mathbf{k},\mathbf{p}_2+\mathbf{k})\rangle \\
& +\frac{Z_1Z_2\alpha}{2\pi^2}\frac{-1}{32m_1^2m_2^2}\int\frac{d\mathbf{k}}{k^2}\langle\phi_0(\mathbf{p}_1,\mathbf{p}_2)|[p_2^2+|\mathbf{p}_2+\mathbf{k}|^2][p_1^2-\mathbf{p}_1\cdot\mathbf{k}-i\boldsymbol{\sigma}_1\cdot(\mathbf{p}_1\times\mathbf{k})]+[p_1^2+|\mathbf{p}_1-\mathbf{k}|^2] \\
& \times[p_2^2+\mathbf{p}_2\cdot\mathbf{k}+i\boldsymbol{\sigma}_2\cdot(\mathbf{p}_2\times\mathbf{k})]-2[p_1^2-\mathbf{p}_1\cdot\mathbf{k}-i\boldsymbol{\sigma}_1\cdot(\mathbf{p}_1\times\mathbf{k})][p_2^2+\mathbf{p}_2\cdot\mathbf{k}+i\boldsymbol{\sigma}_2\cdot(\mathbf{p}_2\times\mathbf{k})] \\
& -\tfrac{1}{2}(p_1^2+|\mathbf{p}_1-\mathbf{k}|^2)(p_2^2+|\mathbf{p}_2+\mathbf{k}|^2)|\phi_0(\mathbf{p}_1-\mathbf{k},\mathbf{p}_2+\mathbf{k})\rangle
\end{aligned}
$$

Numerical approaches

We would prefer numerical approach

Numerical approaches

Standard methods for atomic calculations

(Relativistic) Many-body perturbation theory

can treat correlation and (relativistic) effects to all orders

no QED effects

Numerical approaches

Standard methods for atomic calculations

(Relativistic) Many-body perturbation theory

can treat correlation and (relativistic) effects to all orders

no QED effects

S-matrix formalism

can treat QED effects to second order

no electron correlation

Numerical approaches

We have developed an alternative numerical procedure for QED calculations

Covariant Evolution Operator technique

Can treat quasi-degeneracy

Similarity with MBPT

Fine structure of heliumlike ions

Z	$^3P_1 - ^3P_0$	$^3P_2 - ^3P_0$	$^3P_2 - ^3P_1$	
9	701(10) μH		4364,517(6)	Expt'l
	680	5050	4362(5)	Drake
	690	5050	4364	Göteborg
10	1371(7)	8458(2)		Expt'l
	1361(6)	8455(6)	265880	Drake
	1370	8460	265880	Göteborg
18		124960(30)		Expt'l
		124810(60)		Drake
		124940		Göteborg

I. Lindgren, S. Salomonson, and B. Åsén, Physics Rep. 389, 161 (2004)

Goal

Our goal is to merge the covariant-evolution-operator procedure with the well-established many-body perturbation technique

Covariant relativistic MBPT procedure

Question

How can this be done?

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:

Dirac-Coulomb Approximation

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

Dirac-Coulomb-Breit Approximation

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

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

Instantaneous Breit interaction

Std relativistic MBPT

Std relativistic MBPT:

Dirac-Coulomb Approximation

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

Dirac-Coulomb-Breit Approximation

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

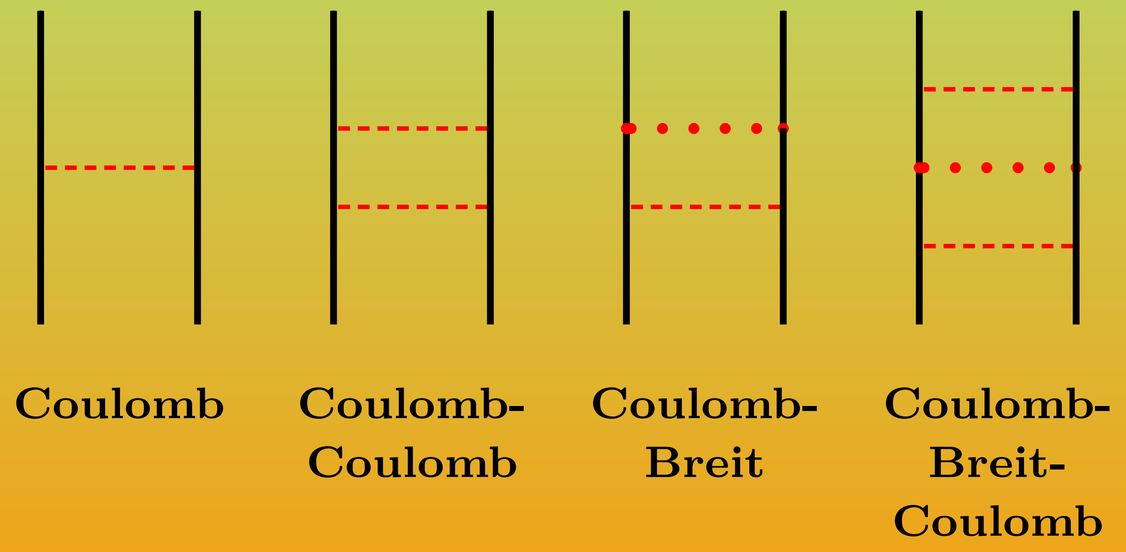
No QED effects

Not relativistically covariant

Correct to order α^2

Std relativistic MBPT

Diagrammatic representation of
Dirac-Coulomb-Breit
for He-like systems

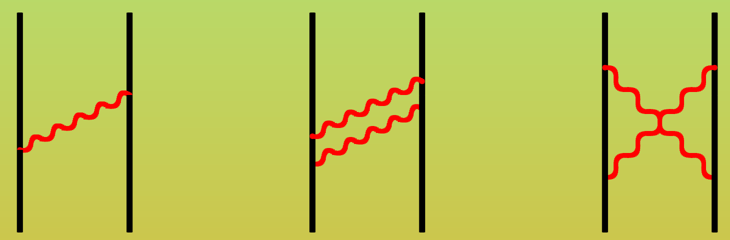


QED effects

QED effects—effects beyond Dirac-Coulomb-Breit

(order α^3 and higher)

Non-radiative effects (retardation, virtual pairs)



Retarded Breit Araki-Sucher

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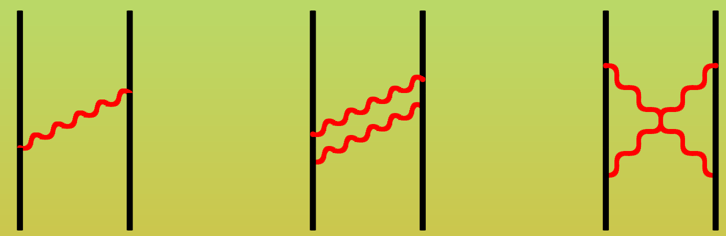
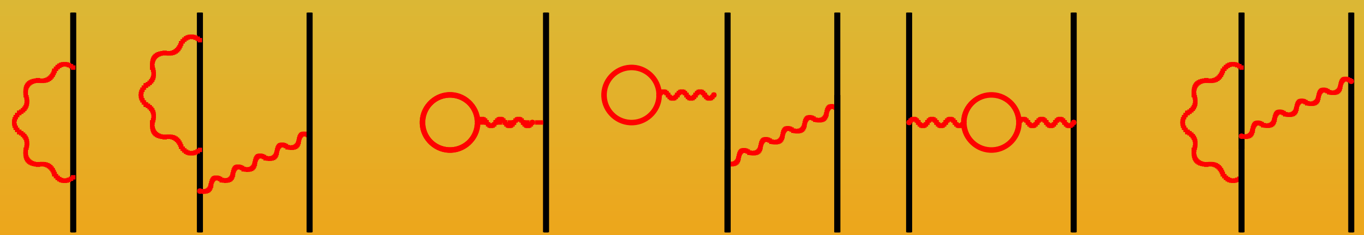


Retarded Breit Araki-Sucher

Radiative effects **(Lamb shift)**



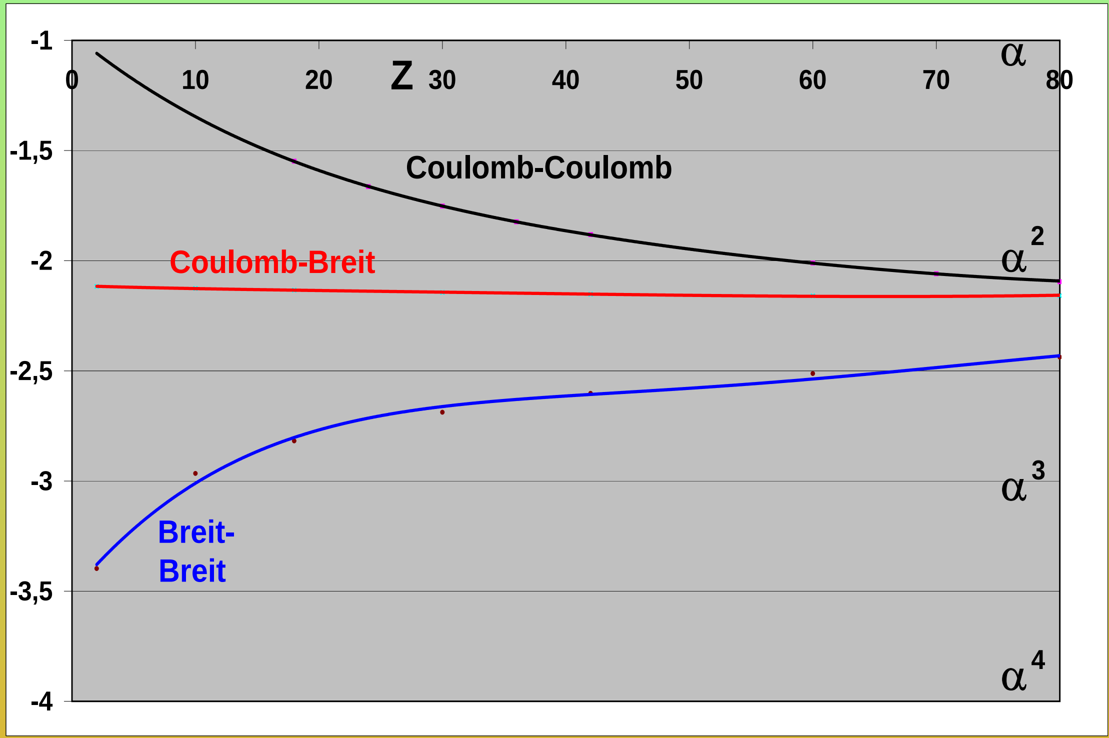
Self energy Vacuum polarization Vertex corr.

Covariant relativistic procedure

A covariant many-body procedure should include all many-body and QED effects

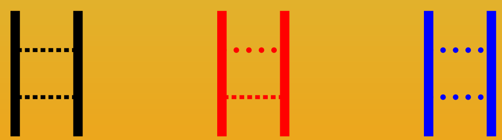
Requires field-theoretical approach

He-like ions



Dirac – Coulomb – Breit

Coul-Coul Coul-Breit Breit-Breit



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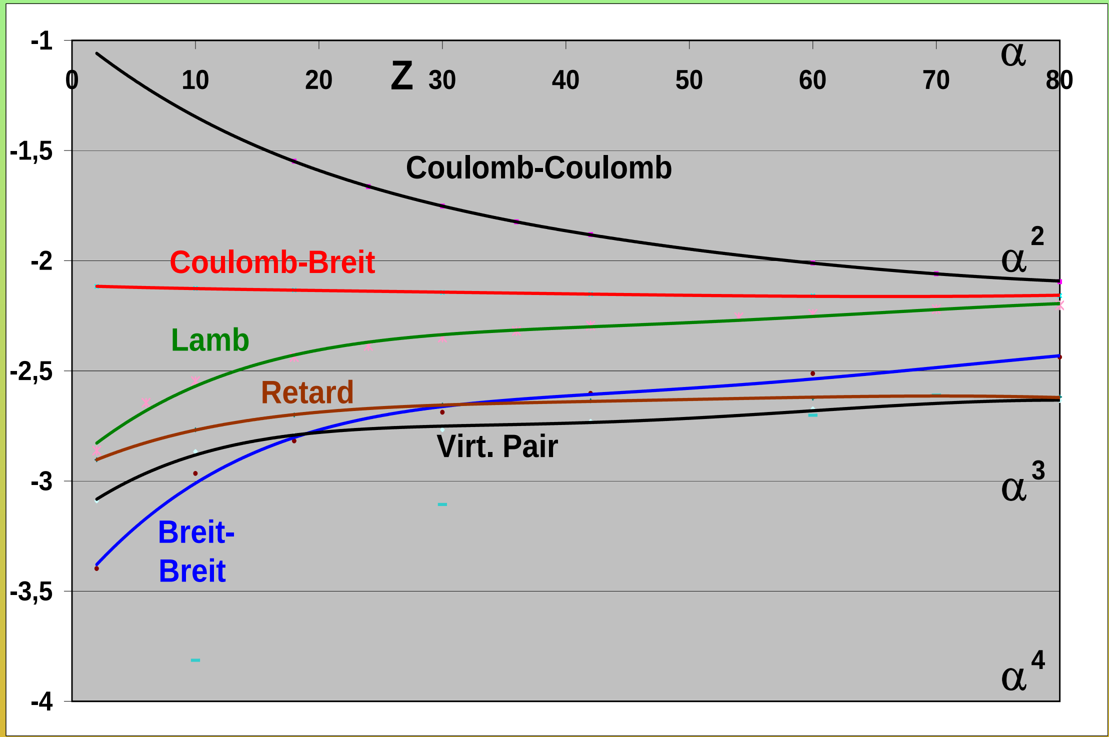
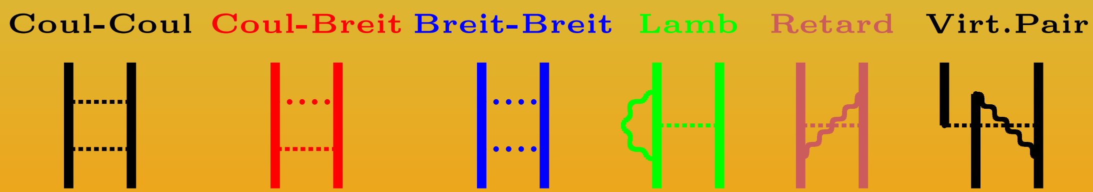
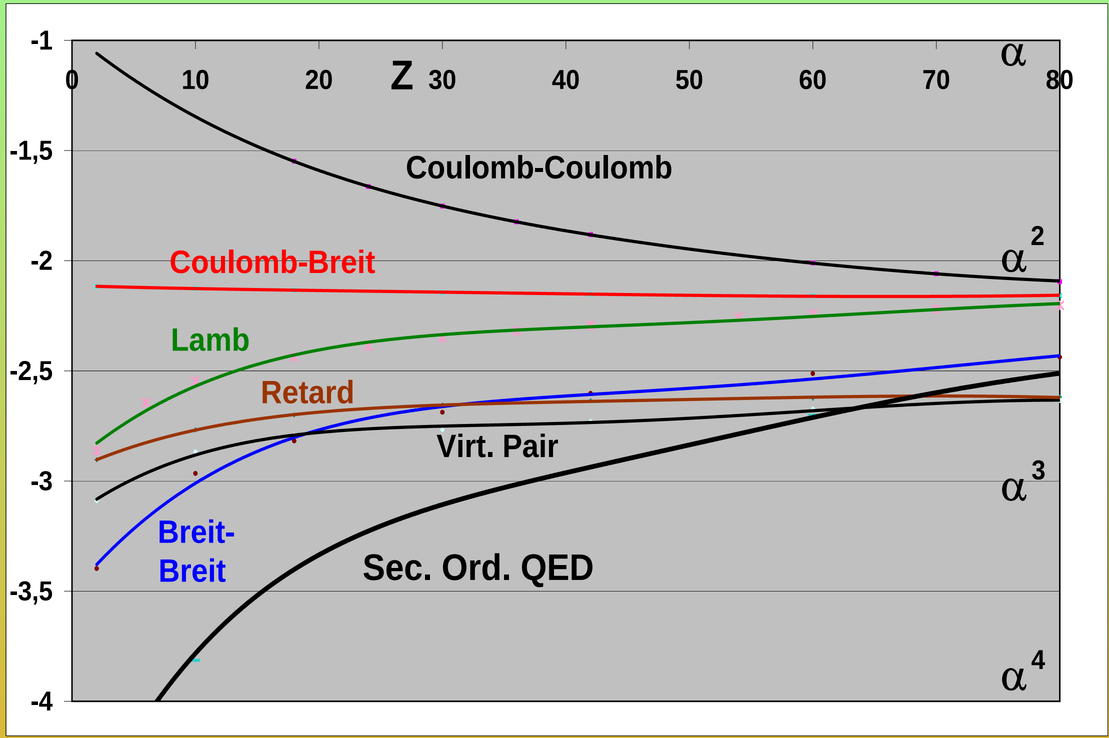


Dirac – Coulomb – Breit

First-order QED



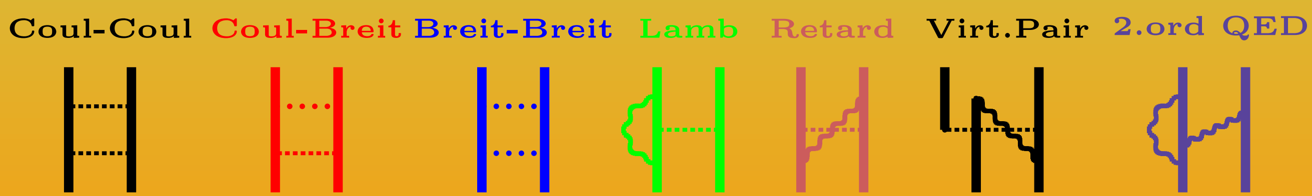
He-like ions



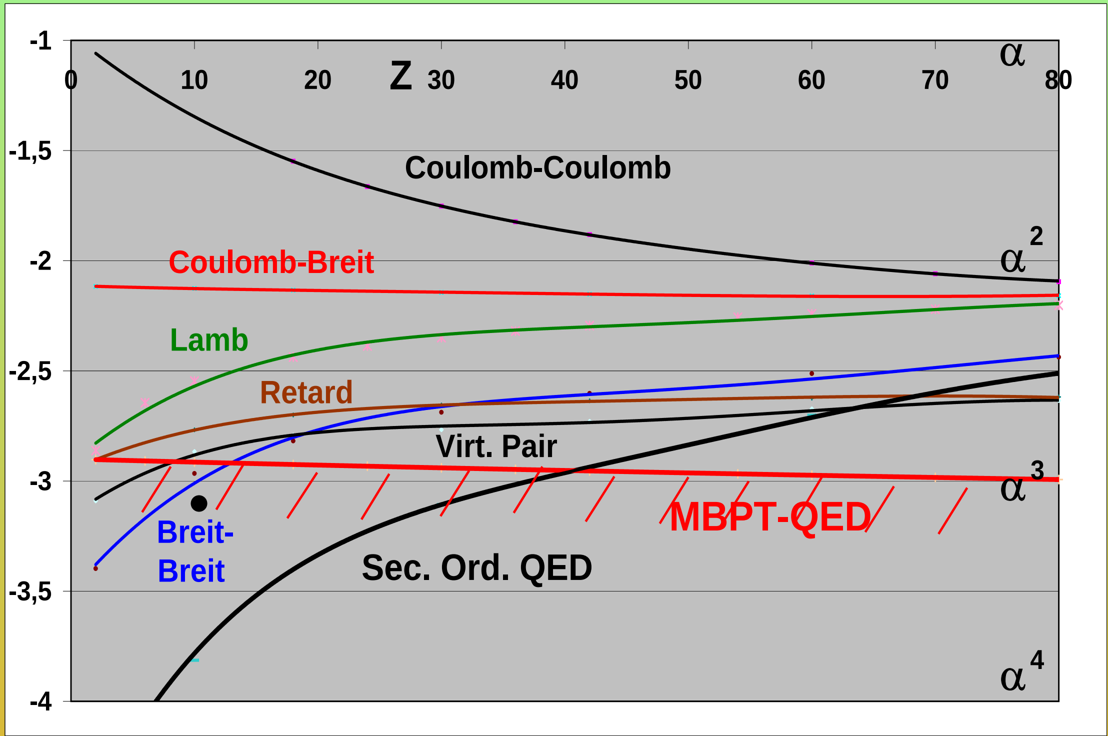
Dirac – Coulomb – Breit

First-order QED

Sec. – order QED



He-like ions



Dirac – Coulomb – Breit

First-order QED

Sec. – order QED

MBPT – QED

First relativistically covariant theory:

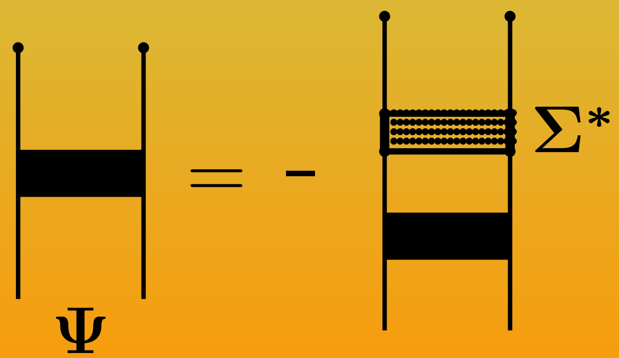
Bethe-Salpeter eqn

Salpeter and Bethe 1951; Gell-Mann and Low 1951

$$\Psi(x,x') = -\iiiint d^4x_1\, d^4x_2\, d^4x_1'\, d^4x_2'$$

$$\times G_0(x,x';x_2,x_2')\,\Sigma^*(x_2,x_2';x_1,x_1')\,\Psi(x,x')$$

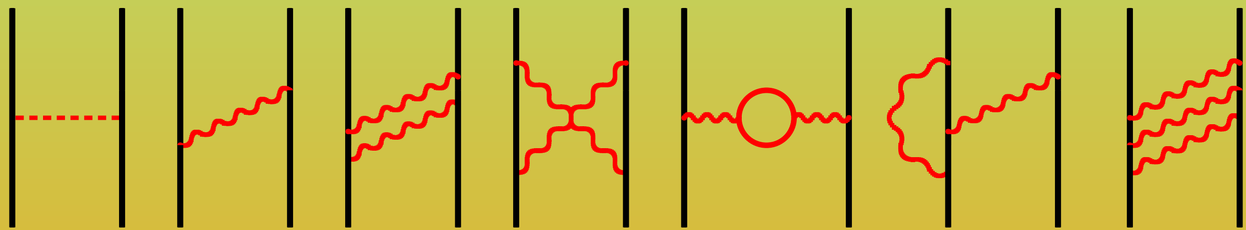
Based on field theory



Bethe-Salpeter equation

"Proper" self-energy represented by all irreducible interaction diagrams

$\Sigma^* =$



$\cdots$

Bethe-Salpeter equation

In principle, the BSE has separate times for the particles

$$\Psi(x, x') = \Psi(t, x, y, z; t', x', y'z')$$

Bethe-Salpeter equation

In principle, the BSE has separate times for the particles

$$\Psi(x, x') = \Psi(t, x, y, z; t', x', y'z')$$

Equal-time approximation: $t = t'$

leads to Schrödinger-like eqn

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

$\mathcal{V}(E) = \Sigma^*(E)$ Effective potential

Bethe-Salpeter equation

BSE can be solved by means of Brillouin-Wigner PT

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

$$Q\Psi(E) = \frac{Q}{E-H_0}\Psi(E)$$

$$\Psi(E) = \left[1 + \frac{Q}{E-H_0}\mathcal{V}(E) + \frac{Q}{E-H_0}\mathcal{V}(E)\frac{Q}{E-H_0}\mathcal{V}(E) + \cdots\right]\Psi_0$$

Not useful as base for MBPT-QED procedure

Covariant evolution operator

Time-dependent perturbation theory

$$H = H_0 + H'(t)$$

Evolution operator

Interaction picture

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

$$\mathrm{i}\frac{\partial}{\partial t}U(t,t_0) = H'(t)U(t,t_0)$$

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

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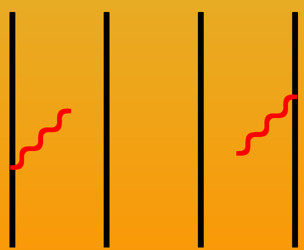


$$\mathcal{H}'(x) = -e\hat{\psi}^{\dagger}\alpha^{\mu}A_{\mu}\hat{\psi}$$

interaction density with the e-m field

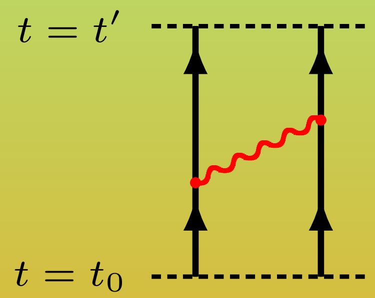
emission and absorp. of virtual photon

Covariant evolution operator

Interaction between the electrons represented by exchange of virtual photons

Evolution operator for single-photon exchange

Contraction of two interactions: $\overbrace{\mathcal{H}'(x_1)\mathcal{H}'(x_2)}$



Time runs only in POSITIVE directions

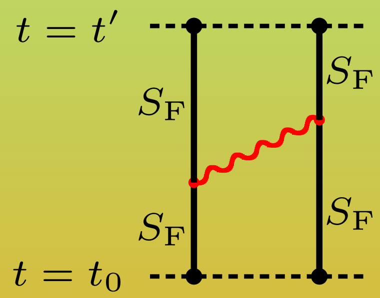
NOT relativistically covariant

Covariant evolution operator

Green's function

contains additional electron propagators

integration over all times



Time runs in BOTH directions

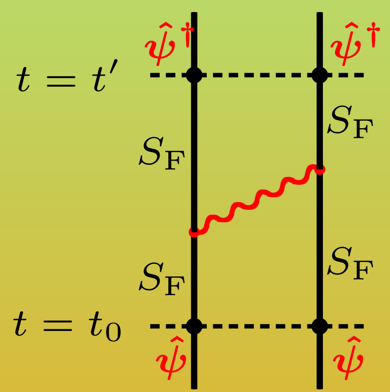
Relativistically covariant

Covariant evolution operator

Covariant evolution operator

contains additional electron-field operators

integration over all times

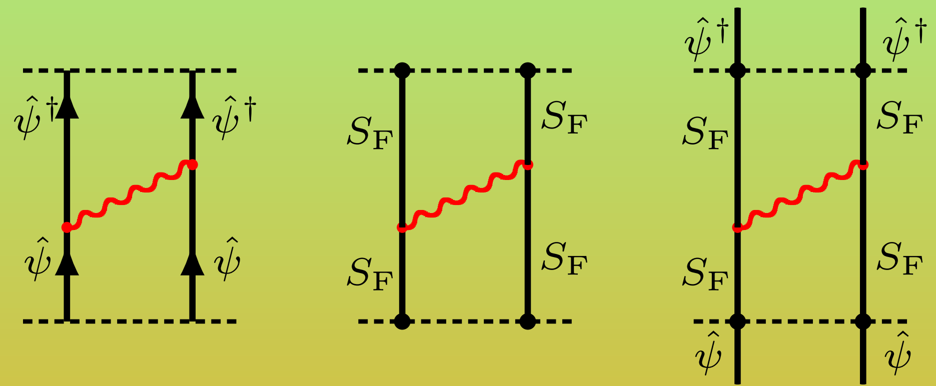


Time runs in BOTH directions

Relativistically covariant

Covariant evolution operator

Std evolution operator — **Green's function** — **Cov. evol. operator**



Not rel. covariant — **Relativistically covariant**

Field-theoretical concepts

Covariant evolution operator

Std evol. operator represents the evolution of the non-relativistic wave function

$$\Psi(t) = U(t, t_0)\, \Psi(t_0)$$

Covariant evolution operator

Cov. evol. operator represents the evolution of the relativistic wave function

$$\Psi_{\mathrm{Rel}}(t) = U_{\mathrm{Cov}}(t, t_0)\, \Psi_{\mathrm{Rel}}(t_0)$$

Covariant evolution operator

Cov. evol. operator represents the evolution of the relativistic wave function

$$\Psi_{\rm Rel}(t) = U_{\rm Cov}(t, t_0)\, \Psi_{\rm Rel}(t_0)$$

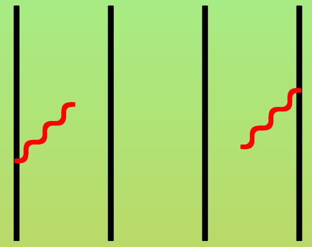
Closely connected to MBPT wave operator

$$\Psi_{\rm Rel} = \Omega\, \Phi_{\rm Rel}$$

I.Lindgren, S.Salomonson, and B.Åsén

Physics Reports, 389, 161 (2004)

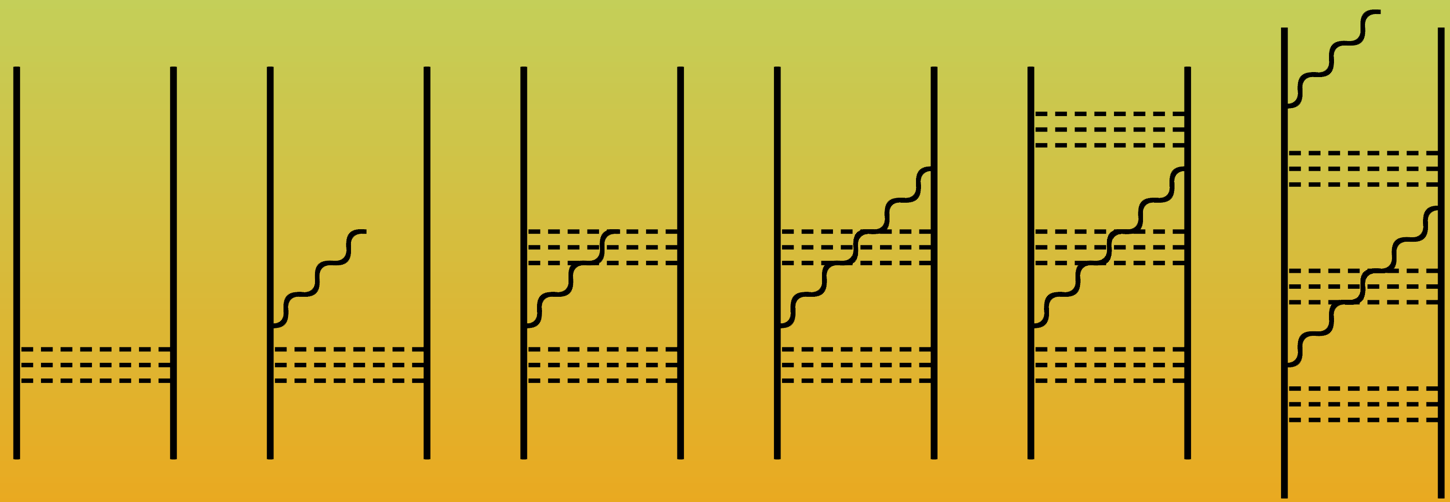
Covariant evolution operator



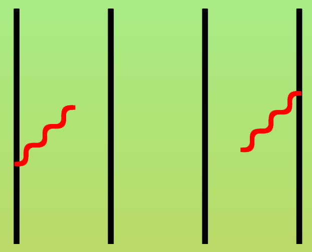
$$\mathcal{H}'(x) = -e\hat{\psi}^\dagger \alpha^\mu A_\mu \hat{\psi}$$

interaction with the e-m field

emission and absorp. of virtual photon



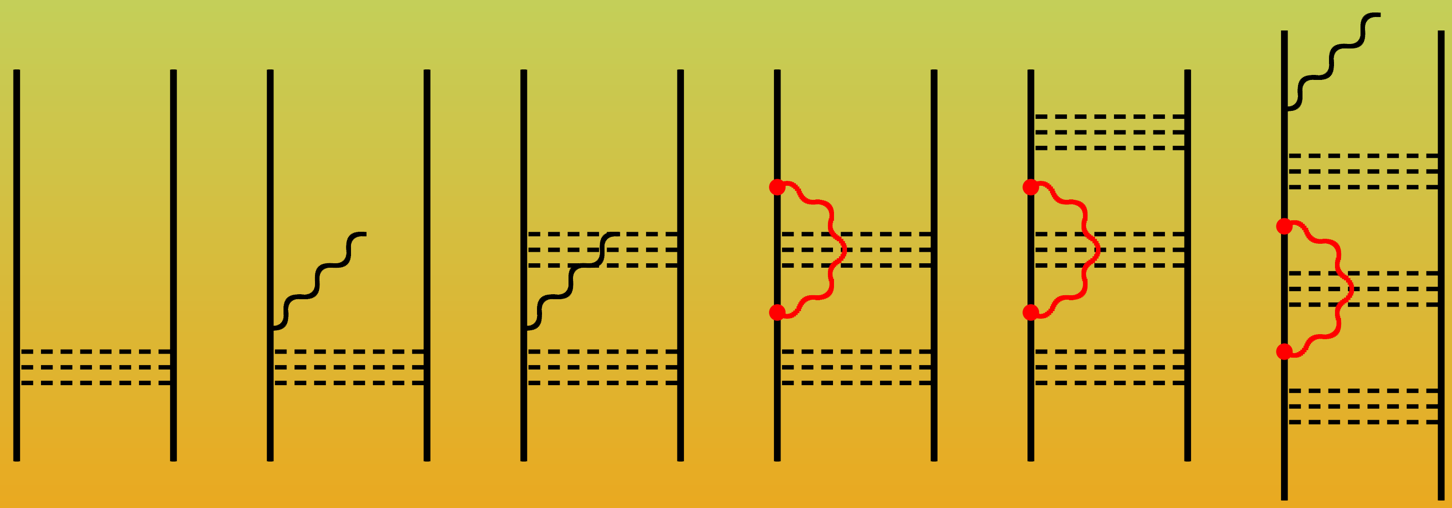
Covariant evolution operator



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

interaction with the e-m field

emission and absorp. of virtual photon



Covariant evolution operator

Leads to the desired field-theoretical form of MBPT

Compatible with Bethe-Salpeter equation

which verifies the relativistic covariance

Compatible with std MBPT

can treat electron correlation to all orders

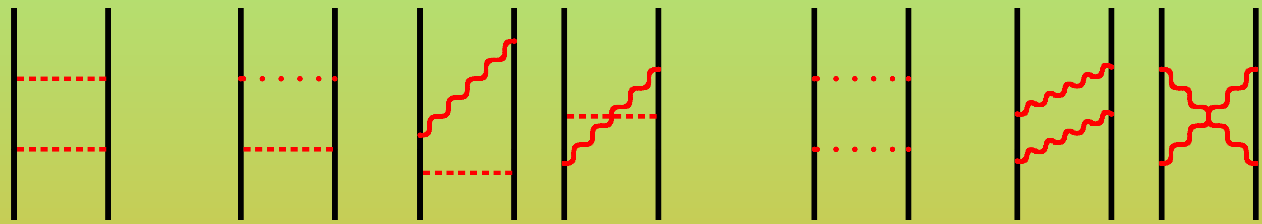
I.Lindgren, S.Salomonson and D.Hedendahl

Can. J. Phys. 83, 183 (2005) "Einstein Centennial paper"

Numerical results

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

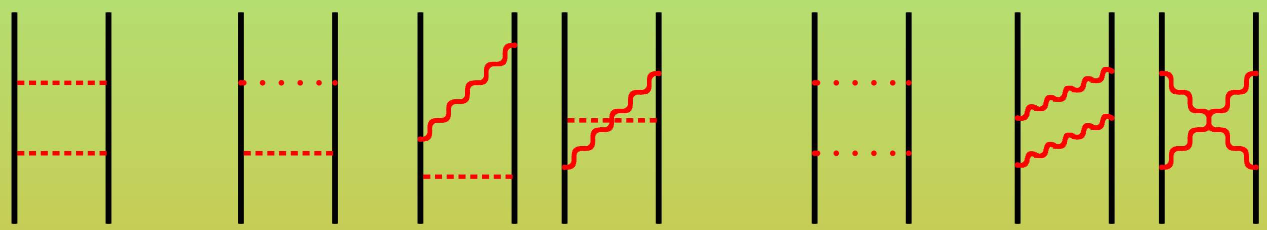
	Coul.-Coul.	Coulomb-Breit unretarded	Coulomb-Breit retard.	Breit-Breit unretard.	Breit-Breit retard.



NVP:	-158 000	-2870	122	-46	13

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

Coul.-Coul. | Coulomb-Breit: unretarded, retard. | B r e i t - B r e i t: unretard., retard.

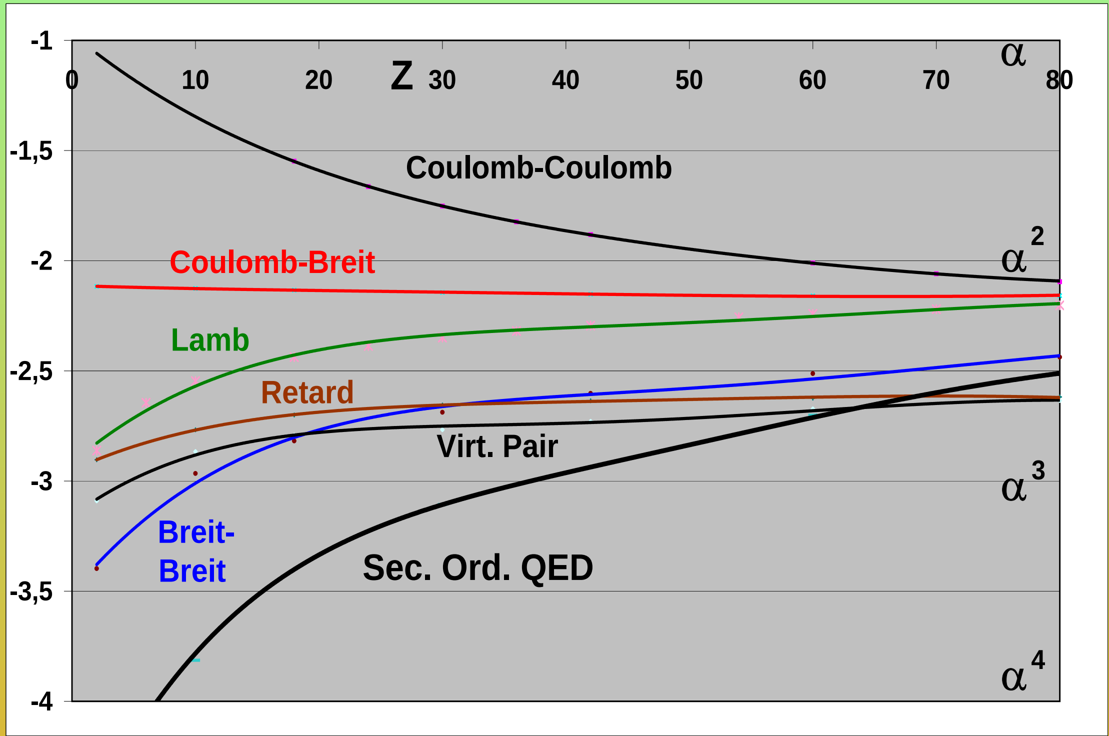


NVP: -158 000 | -2870 | 122 | -46 | 13

+Correlation | +Correlation

-57 | 15 | (2-5)

He-like ions

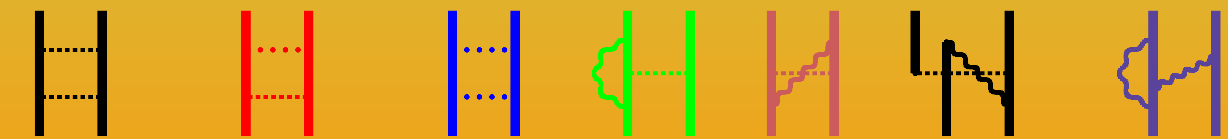


Dirac – Coulomb – Breit

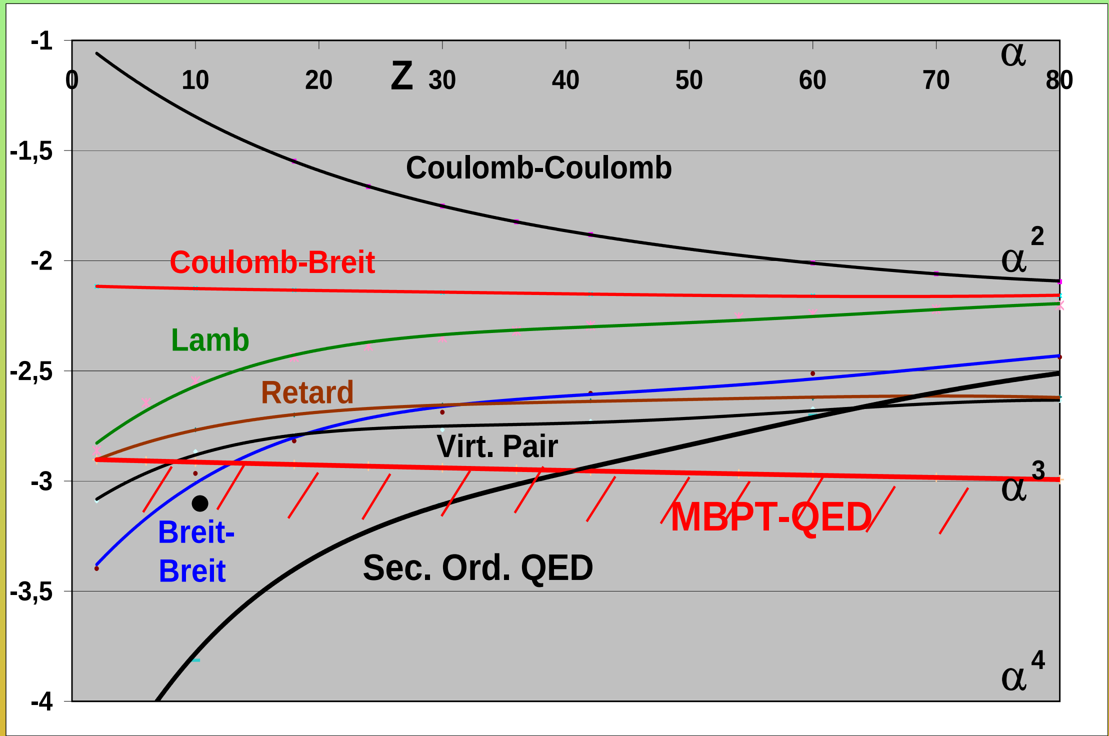
First-order QED

Sec. – order QED

Coul-Coul Coul-Breit Breit-Breit Lamb Retard Virt.Pair 2.ord QED



He-like ions



Dirac – Coulomb – Breit

First-order QED

Sec. – order QED

MBPT – QED

Conclusions

Relativistically covariant MBPT procedure

- **can be constructed by means of Covariant-Evolution-Operator/ Green's-Operator technique**

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Relativistically covariant MBPT procedure

- **can be constructed by means of Covariant-Evolution-Operator/ Green's-Operator technique**

- **Based on Rayleigh-Scbrödinger PT compatible with non-rel linked-diagram procedures**

- **Contains in principle all relativistic and QED effects. Leads for two-electron systems ultimately to Bethe-Salpeter eqn**

Outlook

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- **The new procedure is only partly implemented. Retardation and virtual pairs essentially done, radiative effects (Lamb shift) remain.**
- **It will primarily be used – in conjunction with highly-charged ion experiments – for medium-heavy few-electron ions in order to test the combined MBPT-QED effect.**
- **Particularly challenging are high-accuracy calculations on very light elements (He) in order to resolve the present discrepancy between theory and experiments.**

Fundamental problem

The original Bethe-Salpeter equation:

$$\Psi(x, x') = - \iiiint \mathrm{d}^4 x_1 \, \mathrm{d}^4 x_2 \, \mathrm{d}^4 x'_1 \, \mathrm{d}^4 x'_2$$

$$\times G_0(x, x'; x_2, x'_2) \, \Sigma^*(x_2, x'_2; x_1, x'_1) \, \Psi(x, x')$$

has separate times for the individual particles

$$\Psi(x, x') = \Psi(t, x, y, z; t', x', y' z')$$

Not consistent with std QM picture

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Potential conflict

between field theory and quantum mechanics

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)