Unification of Many-Body Perturbation Theory and Quantum Electrodynamics

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Coworkers

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Daniel Hedendahl
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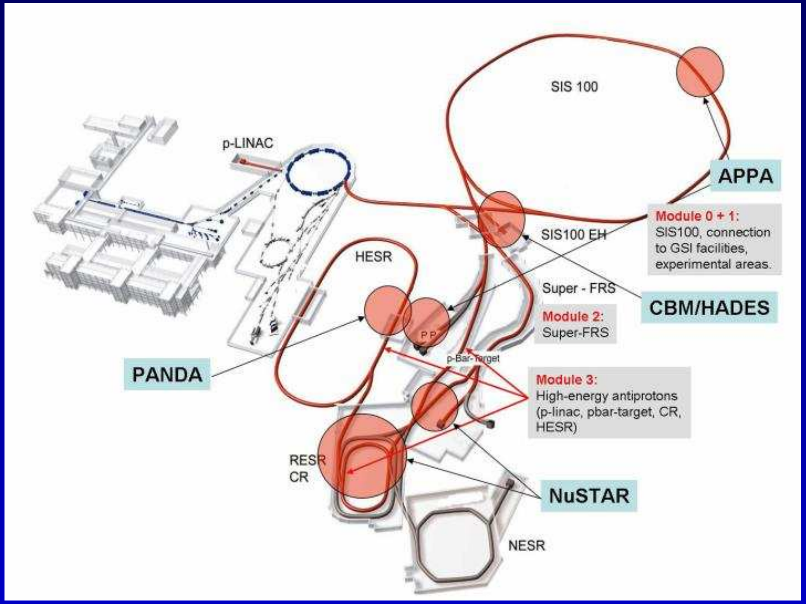
Introduction

Facility for Antiproton and Ion Resear

GSI, Germany



HITRAP

Ion Trap Facility for precision measurements, g-factors

Introduction

Highly charged ions to test QED at strong-fiel

Lamb shift of H-, He-, Li-like ions up to urani

Introduction

Highly charged ions to test QED at strong-fiel

Lamb shift of H-, He-, Li-like ions up to urani

H-like ions less suitable for test of QED
due to large nuclear effect

Introduction

Lamb shift of hydrogenlike uranium (in eV)

Effect	Value
Nuclear size	198.82
First-order self energy	355,05
Vacuum polarization	-88.59
Second-order effects	-1.57
Nuclear recoil	0.46
Nuclear polarization	-0.20
Total theory	**463.95**
Experimental	**460.2 (4.6)**

Introduction

Lamb shift of lithiumlike uranium (in eV)

Effect	Blundell (1993)	Persson (1995)	Yerokh (2002)
Relativistic MBPT	322.41	322.32	322.10
1. order self energy	-53.94	-54.32	
1. ord vacuum pol.	(12.56)	12.56	
1. ord SE + vac. pol.	-41.38	-41.76	-41.77
2. ord SE + vac. pol.		0.03	0.17
Nuclear recoil + pol.	(0.20)	(-0.11)	-0.14
Total theory	**280.83(10)**	**280.54(15)**	**280.48**
Experimental	**280.59(9)**		

Introduction

Transition $1s2s\,^1S_0 - 1s2p\,^3P_1$ (in cm^{-1})

		Reference
Expt'l	**7230.585(6)**	**Myers et al. 2008**
RMBPT	7231	Plante et al. 1994
QED	7229	Artemyev et al. 2005

Plante: All-order rel. MBPT, first-order QED

Artemyev: Second-order QED, first-order correlation

Insufficient

Introduction

Kα lines in Cupper (in eV)

	Kα_1	Kα_2	Reference
Expt'l	**8047.8237(26)**	**8027.8416(26)**	Deslattes et a
Theory	8047.86(4)	8027.92(4)	Chantler et al

From Chantler, Grant et al.

Multi-config. Dirac-Fock with 1. order QED

Insufficient

Levels of MBPT Calculations

Levels of MBPT Calculations

1. Non-relativistic

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

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2. Relativistic No-pair (w. 1. order QED energy)

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

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3. Full QED
Only to second order, not sufficient when correlation important

3a. Unified MBPT-QED Approach

Starts from relativistic no-pair

QED effects to low order included in highly correlated MBPT wave function

Standard non-rel. MBPT:

$$H|\Psi^\alpha\rangle = E^\alpha|\Psi^\alpha\rangle \quad (\alpha = 1\cdots d)$$

$$|\Psi^\alpha\rangle = \Omega|\Psi_0^\alpha\rangle \quad (\alpha = 1\cdots d)$$

Ω wave operator

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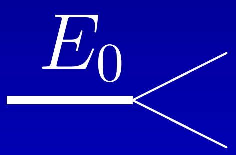
Ω wave operator

Degenerate model space (Bloch 1958)

$$\big(E_0 - H_0\big)\Omega P = Q\big(V\Omega - \Omega V_{\mathrm{eff}}\big)P$$



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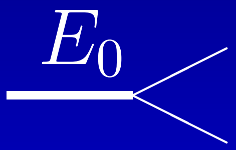
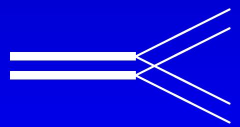


Extended model space (Lindgren 1974)

$$[\Omega, H_0]P = Q\big(V\Omega - \Omega V_{\text{eff}}\big)P$$



Std relativistic MBPT:

Dirac-Coulomb-Breit Approximation

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

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

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

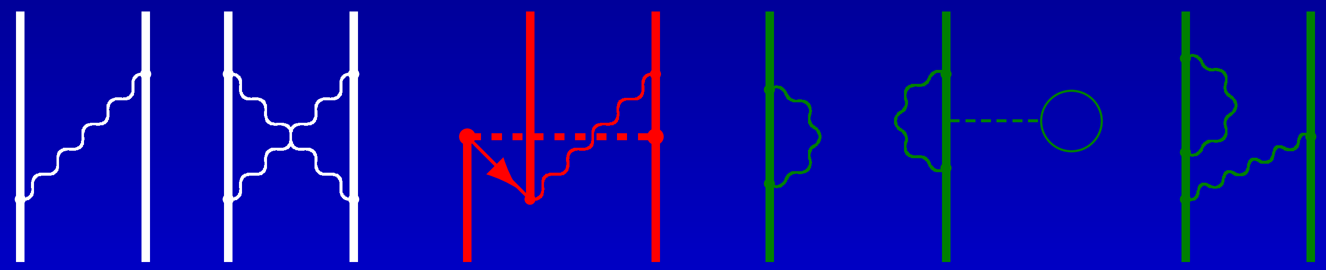
No-Virtual-Pair Approximation (NVPA)

Accurate to order α^2

Effects beyond NVPA

Order α^3 and higher

- **Retardation**
- **Virtual pairs** **Non-radiative**
- **Radiative effects (Lamb shift etc.)**



Non-radiative effects **Radiative effects**

Methods for QED calculations

- **S-matrix (not quasi-degeneracy)**
- **Green's function (St. Petersburg)**
- **Covariant evolution operator (Gothenburg)**

Methods for QED calculations

- **S-matrix (not quasi-degeneracy)**
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Limited to two-photon effects

Not sufficient if correlation important

Feynman gauge

Bethe-Salpeter eqn

First relativistically covariant theory

Salpeter and Bethe 1951; Gell-Mann and Low 1951

Based on field theory

Bethe-Salpeter eqn

First relativistically covariant theory

Salpeter and Bethe 1951; Gell-Mann and Low 1951

Based on field theory

In principle, exact

but not useful for practical work

Unified MBPT-QED Approach

Extension of well-developed MBPT

Unified MBPT-QED Approach

Extension of well-developed MBPT

To go beyond first-order QED

QED has to be included in atomic wave function

Unified MBPT-QED Approach

Extension of well-developed MBPT

First question:

Can QED effects be built into an MBPT expansion?

Never been done before

Unified MBPT-QED Approach

Extension of well-developed MBPT

First question:

Can QED effects be built into an MBPT expansion?

Never been done before

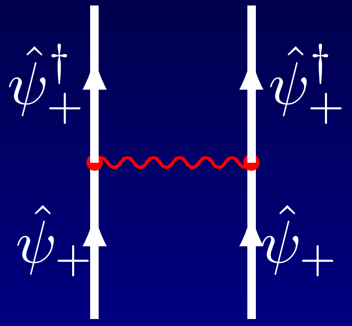
Second question:

Can the QED effects be evaluated using

Coulomb gauge? Never been done before

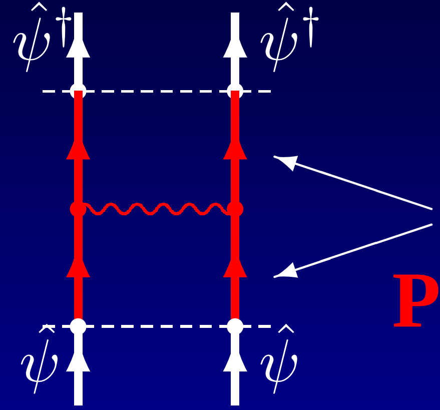
Covariant Evolution Operator (CEO)

Standard



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

Covariant

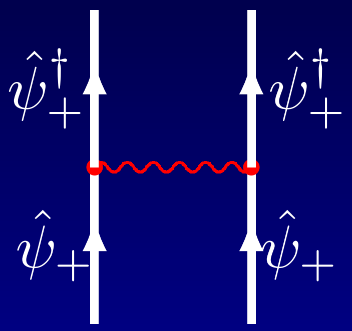


Particles & holes

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

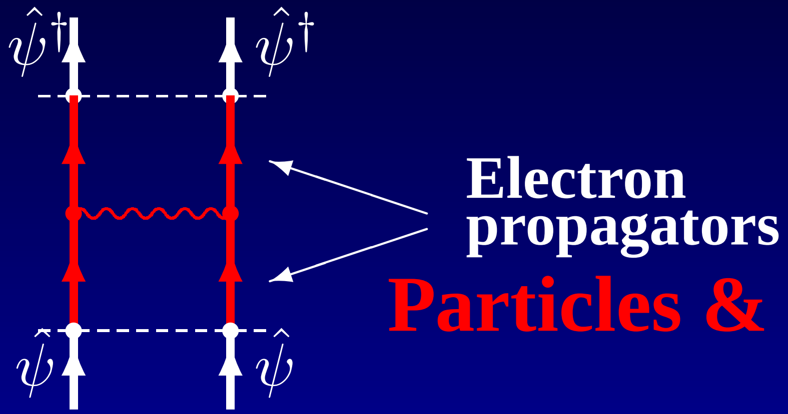
Covariant Evolution Operator (CEO)

Standard



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

Covariant



Particles & holes

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

Covariant evolution operator represents time evolution of relativistic wave function

Green's operator

$$\Psi(t) = U_{\mathrm{Cov}}(t, -\infty)\Phi$$

Φ Parent state

Evolution operator singular

due to intermediate model-space states

Green's operator

$$\Psi(t) = U_{\text{Cov}}(t, -\infty)\Phi$$

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Evolution operator singular

due to intermediate model-space states

$$\Psi(t) = \mathcal{G}(t) \cdot \underbrace{PU_{\text{Cov}}(0, -\infty)\Phi}$$

Model state: $P\Psi(0) = \Psi_0$

$$\Psi(t) = \mathcal{G}(t)\Psi_0$$

Green's operator

$$\Psi(t) = U_{\mathrm{Cov}}(t, -\infty)\Phi$$ Φ Parent state

Evolution operator singular

due to intermediate model-space states

$$\Psi(t) = \mathcal{G}(t) \cdot \underbrace{PU_{\mathrm{Cov}}(0, -\infty)\Phi}$$

Model state: $P\Psi(0) = \Psi_0$

$$\Psi(t) = \mathcal{G}(t)\Psi_0$$

Compare std MBPT: $\Psi = \Omega\Psi_0$

Energy-independent perturbation

$$\left(E_0 - H_0\right)\Omega = Q\left(V\Omega - \Omega V_{\text{eff}}\right)$$

$$\Omega = 1 + \Gamma_Q V\Omega - \Gamma_Q \Omega V_{\text{eff}}$$

$$\Gamma_Q = Q \Big/ \left(E_0 - H_0\right)$$

Energy-independent perturbation

$$(E_0 - H_0)\Omega = Q\left(V\Omega - \Omega V_{\mathrm{eff}}\right)$$

$$\Omega = 1 + \Gamma_Q V \Omega - \Gamma_Q \Omega V_{\mathrm{eff}}$$

$$\Gamma_Q = Q \Big/ (E_0 - H_0)$$

General energy-dependent perturbation

$$\mathcal{G} = 1 + \Gamma_Q V \mathcal{G} + \frac{\delta^* \mathcal{G}}{\delta \mathcal{E}} \mathcal{E} \Big|_{\mathcal{E}=E_0} V_{\mathrm{eff}}$$

Green's operator

$$\Psi(t) = \mathcal{G}(t)\Psi_0$$

$$\Psi = \Omega\Psi_0$$

Green's operator time-dependent wave operat

Connection between field-theoretical CEO and standard MBPT

Coulomb gauge

In combining QED with MBPT

Coulomb gauge has to be used

Coulomb gauge

Perturbation in Coulomb gauge

$$V(t) = V_C + v_T(t)$$

Coulomb + Transverse

Coulomb gauge

Perturbation in Coulomb gauge

$$V(t) = V_C + v_T(t)$$

Coulomb + Transverse

$$V_C = \frac{e^2}{4\pi r_{12}}$$

$$v_T(t) = -\int \mathrm{d}^3x\, \hat{\psi}(x)^\dagger ec\alpha^\mu A_\mu(x)\hat{\psi}(x)$$

Gell-Mann-Low theorem

Schrödinger-like equation in photonic Fock space

$$H_D|\Psi\rangle = \Big(H_0 + V_C + v_T(0)\Big)\,|\Psi\rangle = E\,|\Psi\rangle$$

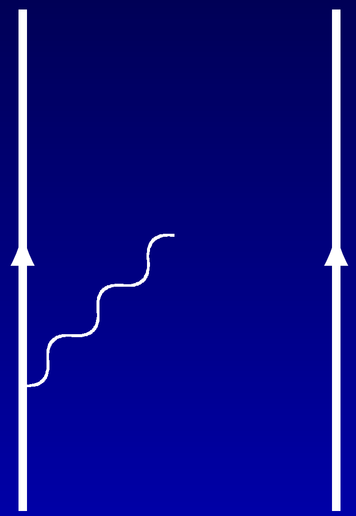
Gell-Mann-Low theorem

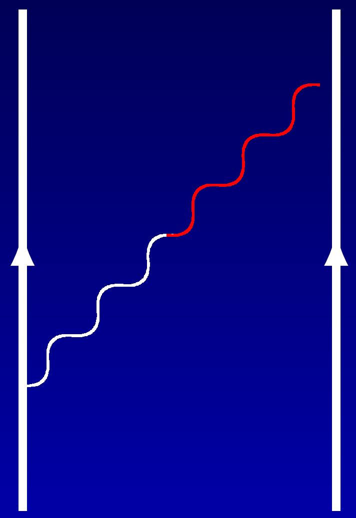
Schrödinger-like equation in photonic Fock space

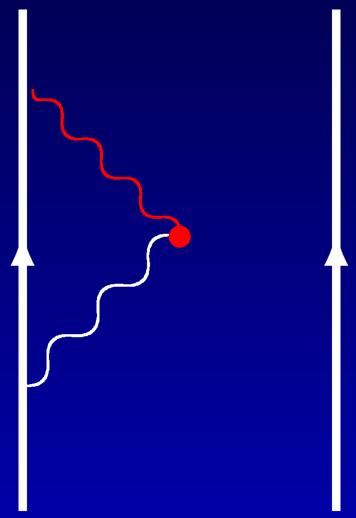
$$H_D|\Psi\rangle = \Big(H_0 + V_C + v_T(0)\Big)\,|\Psi\rangle = E\,|\Psi\rangle$$

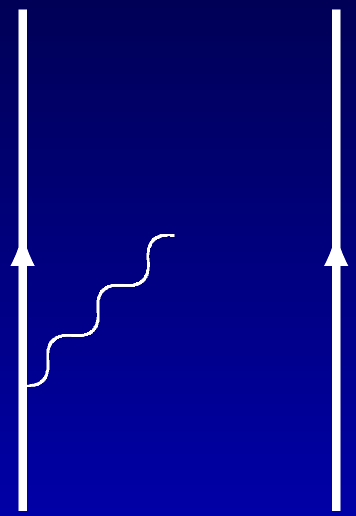
Field-theoretical relation

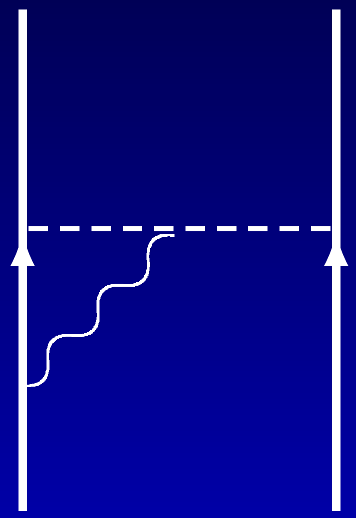
Photonic Fock space

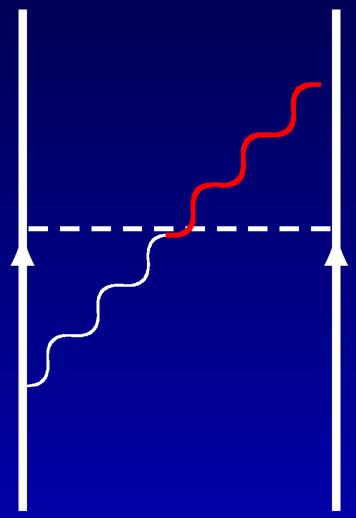


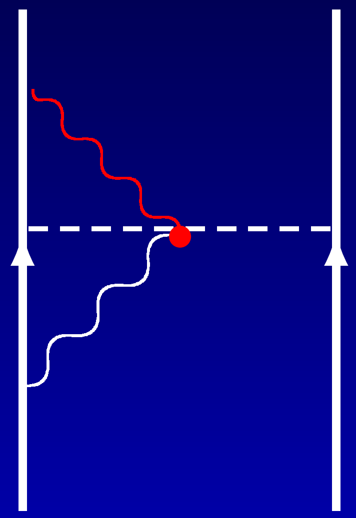




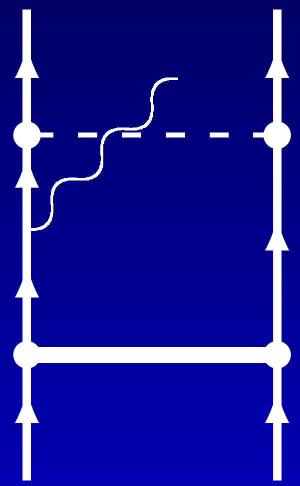




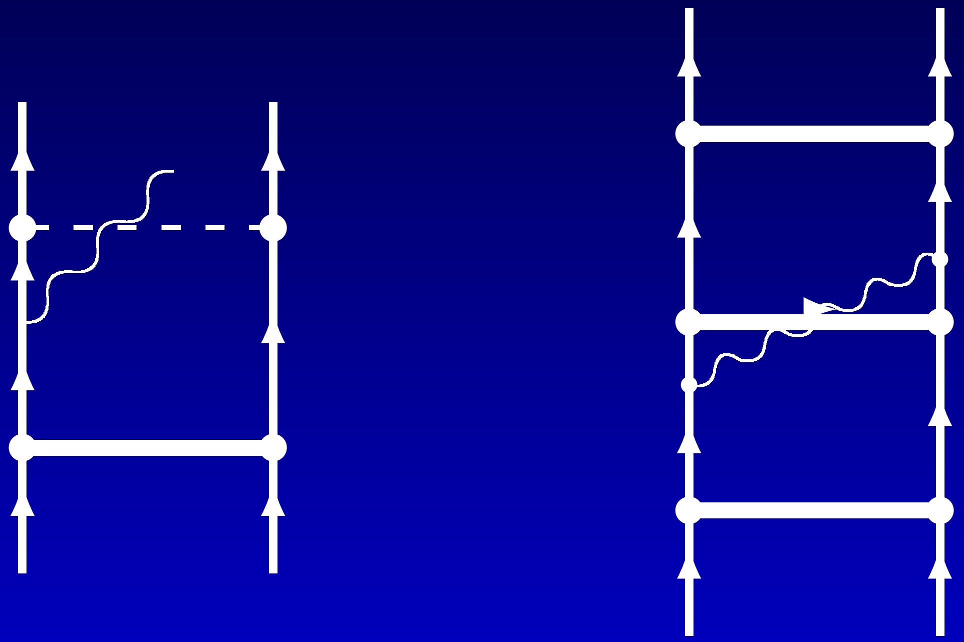




Non-radiative QED with correlation

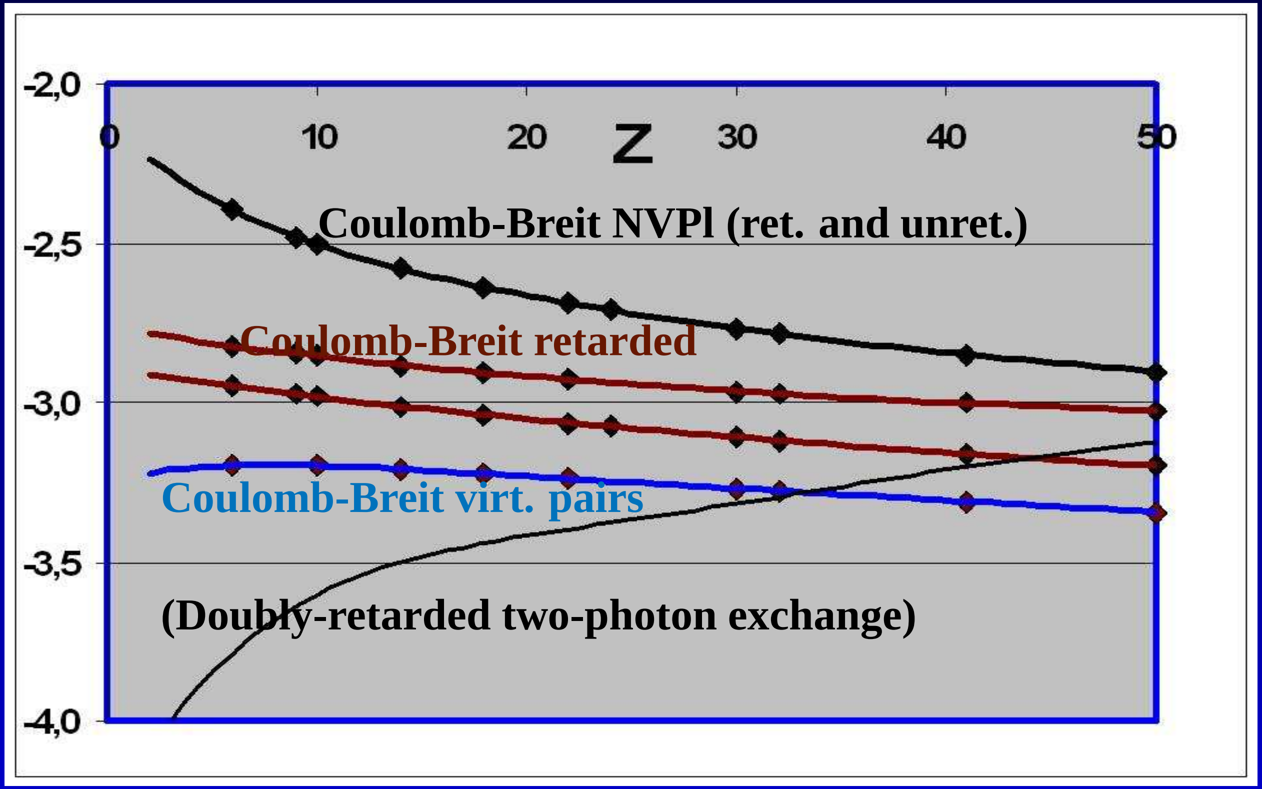


Non-radiative QED with correlation



First-order non-rad. QED with correla

Beyond two-photon exchange



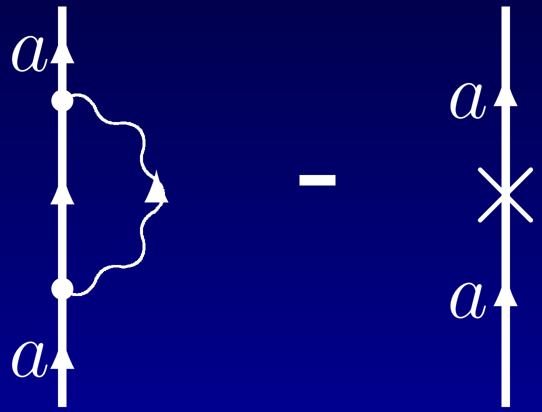
Daniel Hedendahl's PhD thesis 2010

First-order non-rad. QED with correla

First-order non-radiative QED with correlation beyond second order more important than pure second-order QED for light and medium-heavy elements

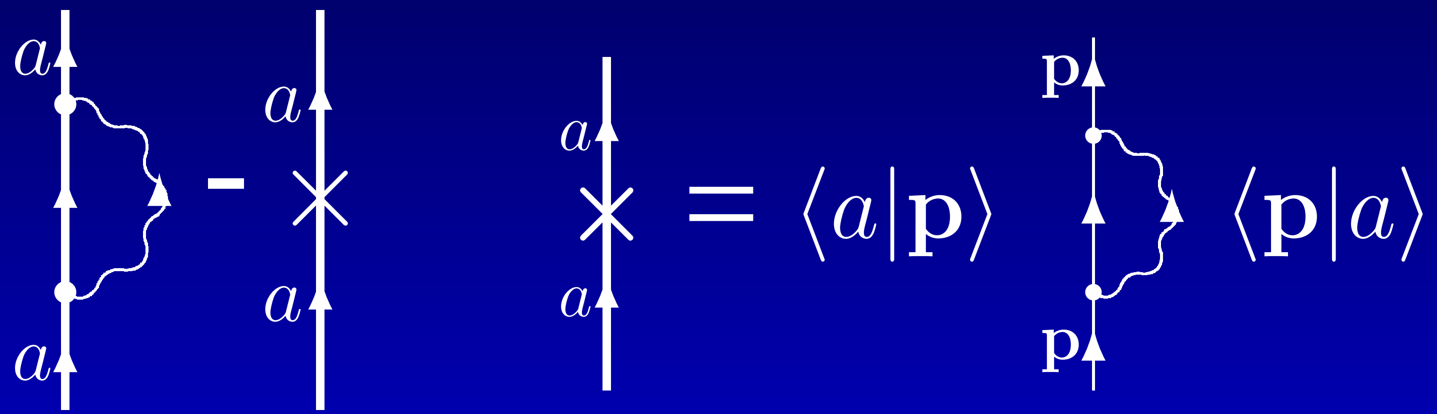
Radiative QED

Mass renormalization



Radiative QED

Partial-wave regularization



Free-electron mass term equals self-energy on the mass shell

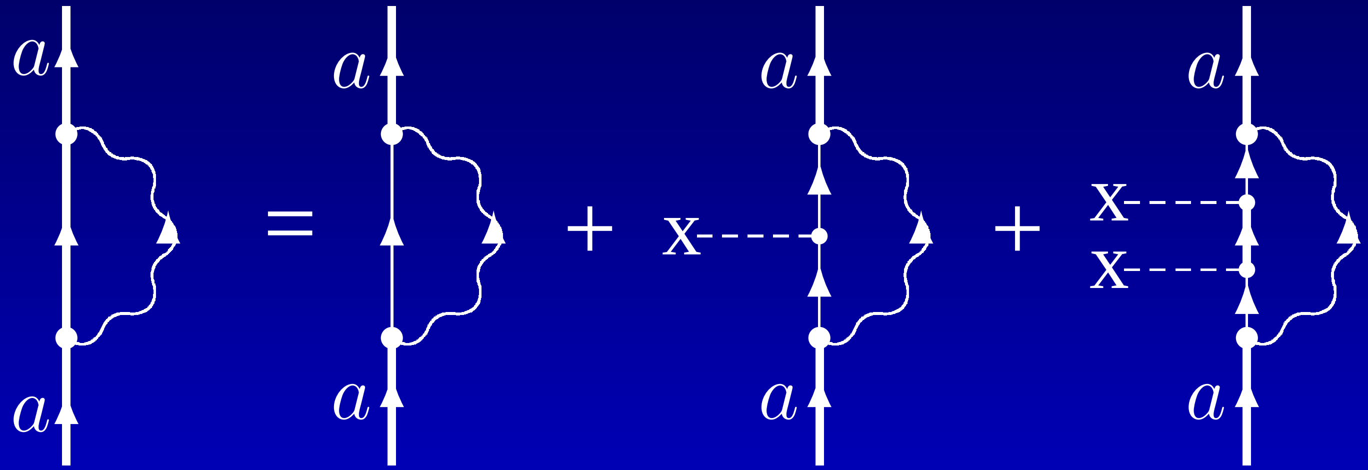
$$\delta m^{\mathrm{free}} = \Sigma^{\mathrm{free}}(p)_{\not p = m}\,; \quad p_0 = \varepsilon_p$$

$$\delta m^{\mathrm{bound}} = \langle a|p\rangle\langle p|\Sigma^{\mathrm{free}}(p)_{\not p = m}|p\rangle\langle p|a\rangle$$

Does not work in Coulomb gauge

Radiative QED

Dimensional regularization



Zero- and one-potential terms evaluated by means of Adkins formulas modified by Johan Holmberg in his Master Thesis

Many-potential term by evaluating the other terms with partial-wave expansion

Radiative QED

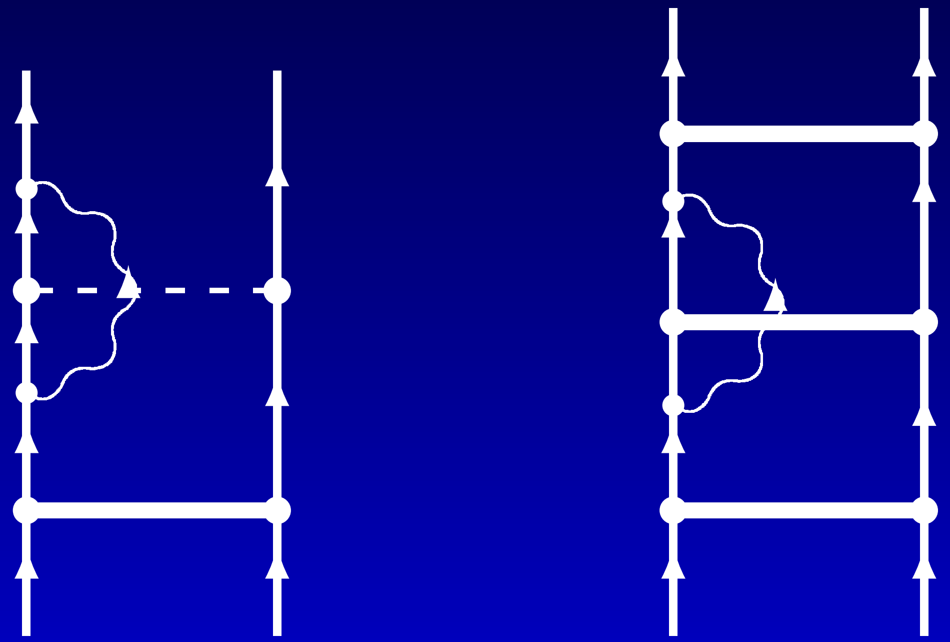
Self-energy of hydrogen like ions

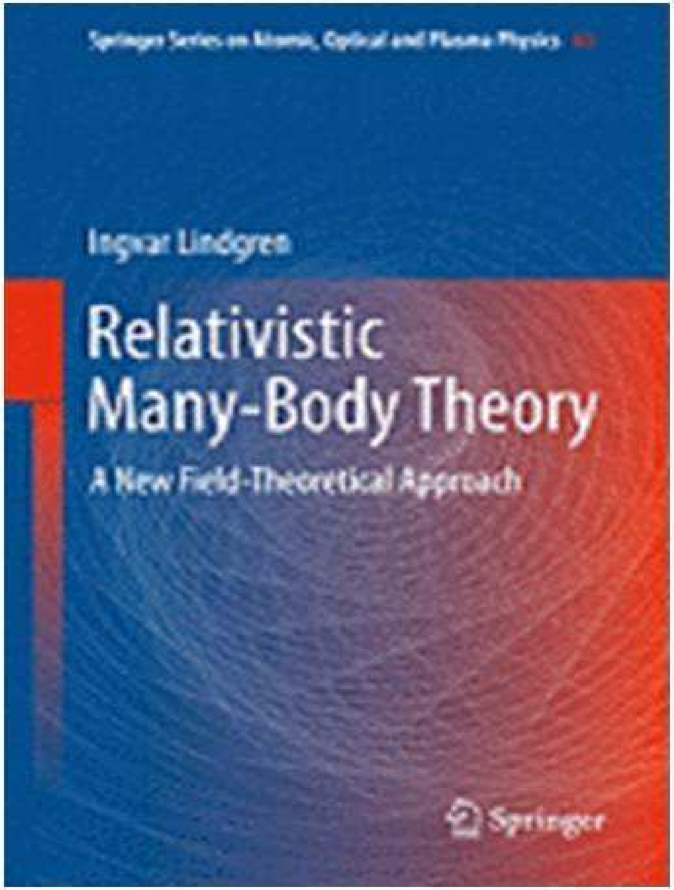
Z	Coulomb gauge	Feynman gauge
18	1.216901(3)	1.21690(1)
54	50.99727(2)	50.99731(8)
66	102.47119(3)	102.4713(1)
92	355.0430(1)	355.0432(2)

First numerical application in Coulomb gauge

D. Hedendahl and J. Holmberg, Phys. Rev. A (accepted)

Non-radiative QED with correlation

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