Unifying Quantum Electrodynamics and Many-Body Perturbation Theory

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New Horizons in Physics

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In honor of Prof. Walter Greiner
at his 80^{th} birthday

Coworkers

Sten Salomonson

Daniel Hedendahl

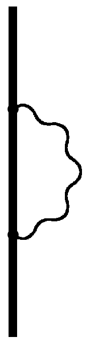
Johan Holmberg

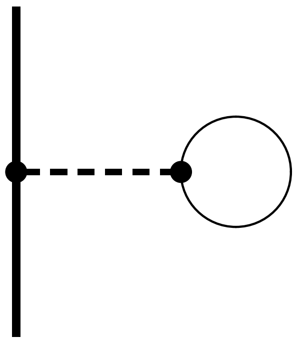
Combining MBPT and QED

Quantum physics/chemistry follows mainly

the rules of Quantum Mechanics (QM)

Some effects lie outside: Lamb shift
(electron self-energy and vacuum polarization)





Combining MBPT and QED

Quantum physics/chemistry follows mainly

the rules of Quantum Mechanics (QM)

Some effects lie outside: Lamb shift
(electron self-energy and vacuum polarization)

require Field theory (QED)

Normally these effects are evaluated separately
For high accuracy they should be evaluated in a
coherent way

QED effects should be included in the
wave function

Combining MBPT and QED

QM and QED are seemingly

incompatible

QM: single time $\Psi(t, \boldsymbol{x}_1, \boldsymbol{x}_2, \cdots)$

Field theory: individual times $\Psi(t_1, \boldsymbol{x}_1; t_2, \boldsymbol{x}_2, \cdots)$

Consequence of relativistic covariance

Bethe-Salpeter equation is

relativistic covariant

can lead to spurious solutions

(Nakanishi 1965; Namyslowski 1997)

Combining MBPT and QED

Compromise:

Equal-time approximation

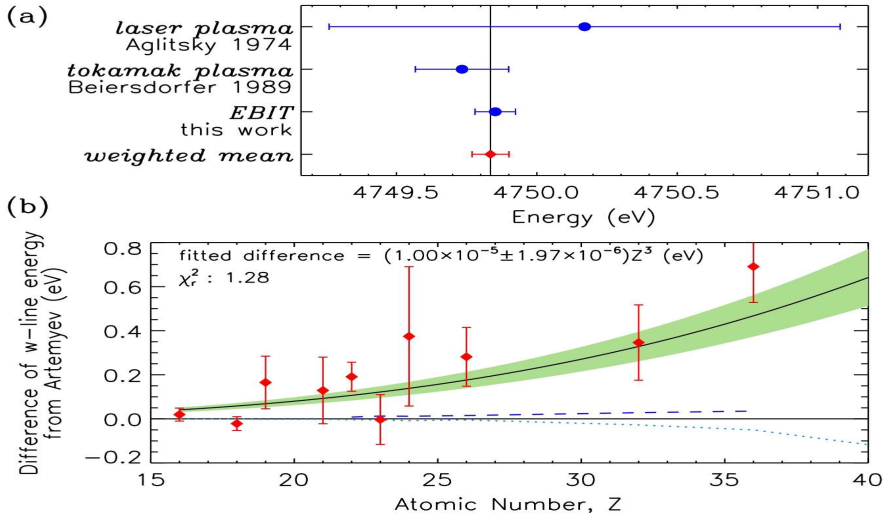
All particles given the same time

makes FT compatible with QM

Some sacrifice of the full covariance

very small effect at atomic energies

Controversy



Chantler (2012) claims that there are significant discrepancies between theory and experiment for X-ray energies of He-like ions

Theory: Artemyev et al 2005, Two-photon QED

Higher-order QED

Higher -order QED can be evaluated by means of the procedure for

combining QED and MBPT using the **Green's operator,**

a procedure for **time-dependent perturbation theory**

Time-independent perturbation

$$H\Psi = (H+V)\Psi = E\Psi \quad \text{target function}$$

$$\Psi_0 = P\Psi \quad \text{model function}$$

P projection operator for the model space

$$\Psi = \mathbf{\Omega}\Psi_0 \quad \mathbf{\Omega} \textbf{ wave operator}$$

Bloch equation

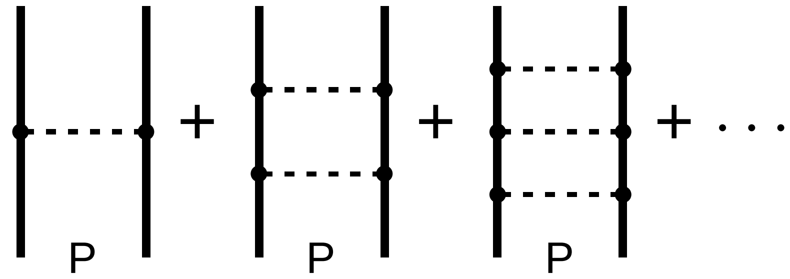
$$\mathbf{\Omega}P = \Gamma\big(V\mathbf{\Omega} - \mathbf{\Omega}W\big)P \qquad \Gamma = \frac{1}{E_0 - H_0}$$

$$W = PV\mathbf{\Omega}P \quad \textbf{Effective Interaction}$$

$$H_{\text{eff}}\Psi_0 = (PH_0P + W)\Psi_0 = (E_0 + \Delta E)\Psi_0 \quad \text{Effective Ham.}$$

Bloch equation

$$\Omega P = \Gamma\big(V\Omega - \Omega W\big)P \qquad \Gamma = \frac{1}{E_0 - H_0}$$

$\Gamma V \Omega P =$ 

$$= [\Gamma V + \Gamma V \Gamma V + \Gamma V \Gamma V \Gamma V + \cdots]P$$

Singular when intermediate state in model space (P)

Singularity cancelled by the term $-\Gamma\Omega W P$

Leads to **Bloch equation**

$$\Omega P = \Gamma_Q\big(V\Omega - \Omega W\big)P \qquad \Gamma_Q = \frac{Q}{E_0 - H_0}$$

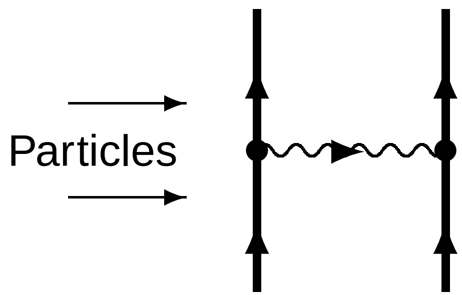
The finite remainder is the

Model-Space Contr. $-\Gamma_Q \Omega W P$

Time-dependent perturbation

Standard time-evolution operator

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

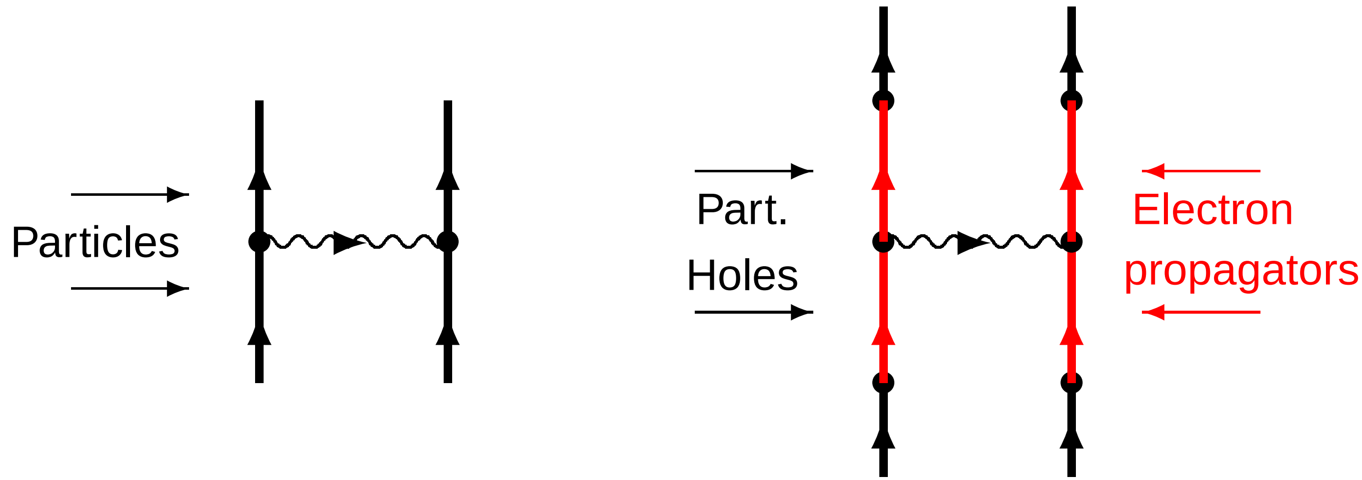


Time propagates only forwards

Time-dependent perturbation

Standard time-evolution operator

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

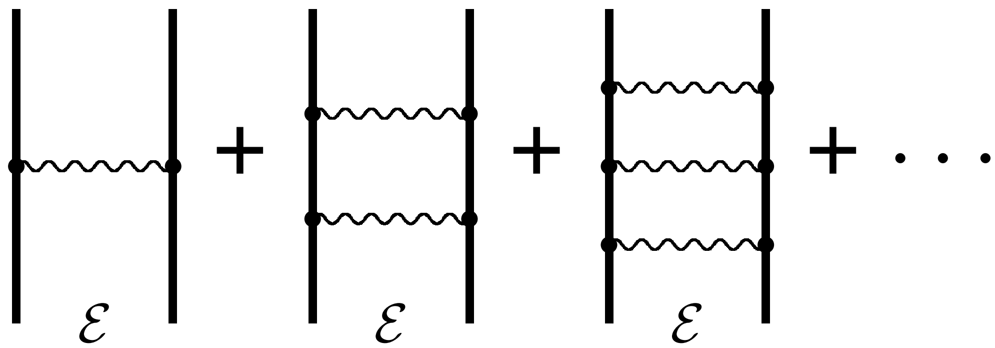


Electron propagators make evolution operator **covariant**

Covariant Evolution Operator (U_{Cov})

Time-dependent perturbation

Covariant evolution ladder $(t = 0,\ t_0 = -\infty)$

$U_{\mathrm{Cov}} = 1 +$ 

$$U_{\mathrm{Cov}} = 1 + \Gamma V + \Gamma V \Gamma V + \cdots \;; \qquad \Gamma = \frac{1}{\mathcal{E} - H_0}$$

Same as first part of MBPT wave operator

$$\boldsymbol{\Omega} = 1 + \Gamma\big(V\boldsymbol{\Omega} - \boldsymbol{\Omega} W\big)$$

Singular when intermediate state in model space

Green's operator

The **Green's operator** is defined

$$U_{\mathrm{Cov}}(t) = \mathcal{G}(t) \cdot P U_{\mathrm{Cov}}(0)$$

is the **regular part** of the Covariant Evolution Oper.

Green's operator

$\underline{\underline{t=0}}$: First order: $\mathcal{G}^{(1)} = U^{(1)}_{\text{Cov}} = \Gamma_Q V = \Omega^{(1)}$

Second order:

$$\mathcal{G}^{(2)} = \Gamma_Q V \mathcal{G}^{(1)} + \frac{\delta \mathcal{G}^{(1)}}{\delta \mathcal{E}} W^{(1)} \, ; \qquad \Gamma_Q = \frac{Q}{\mathcal{E} - H_0}$$

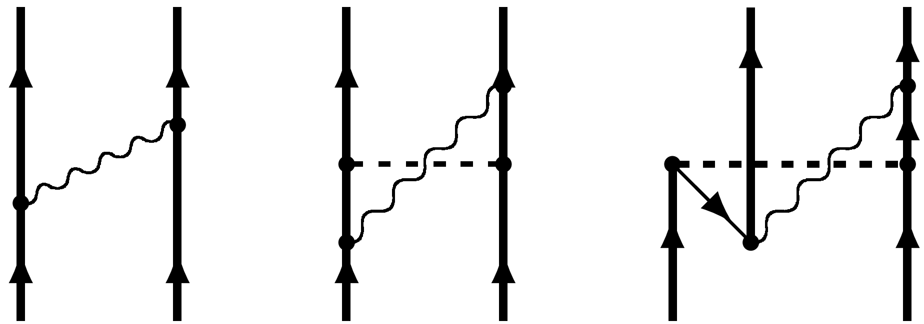
$$= \Gamma_Q V \mathcal{G}^{(1)} - \Gamma_Q \, \mathcal{G}^{(1)} \, W^{(1)} + \boxed{\Gamma_Q \, \frac{\delta V}{\delta \mathcal{E}} W^{(1)}}$$

$$\Omega^{(2)} = \Gamma_Q V \Omega^{(1)} - \Gamma_Q \Omega^{(1)} W^{(1)}$$

Time- or energy-dependent perturbations can be included in the wave function

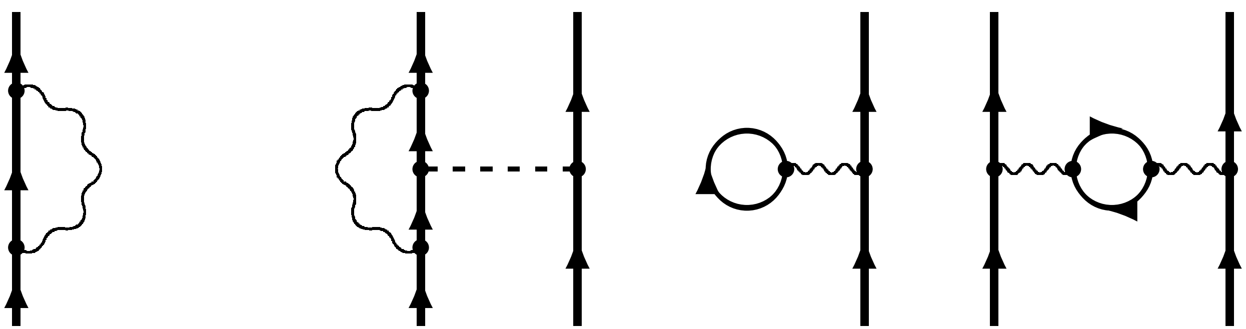
QED effects

Non-radiative



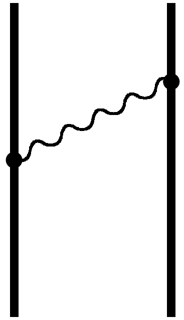
Retardation　　　　Virtual pair

Radiative



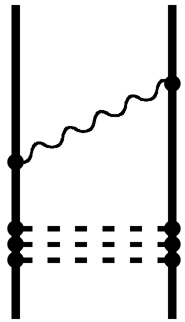
El. self-energy　　Vertex correction　　Vacuum polarization

QED effects are time dependent

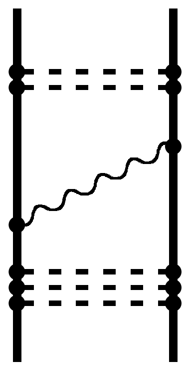


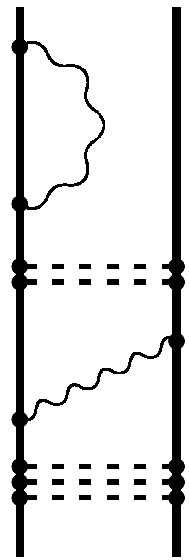
QED effects are time dependent

Can be combined with electron correl.



Continued iterations





Mixing time-independent and time-dependent perturbat.

Combining QED and MBPT

Radiative QED

Dimensional regularization in Coulomb gauge

Developed in the 1980's for Feynman gauge

Formulas for Coulomb gauge derived by Atkins in the 80's

Workable procedure developed by Johan Holmberg in 2011

First applied by Holmberg and Hedendahl

Self-energy of hydrogen like ions

Hedendahl and Holmberg, Phys. Rev. A 85, 012514 (2012)

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)**

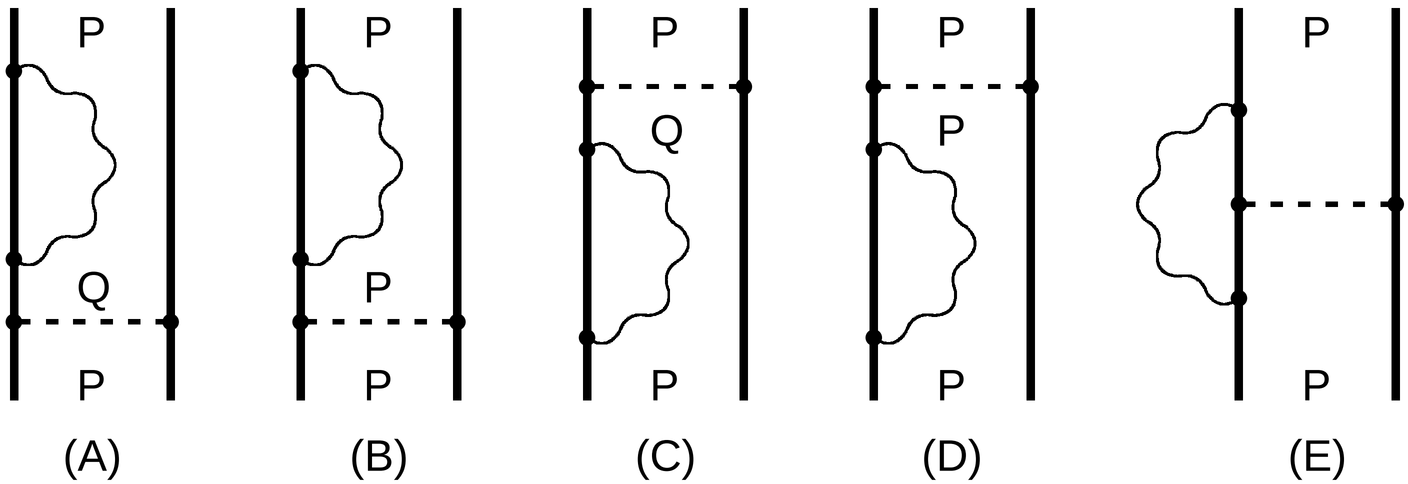
$$\Delta E = \frac{\alpha}{\pi} \frac{(Z\alpha)^4\, mc^2}{n^3}\; F(Z\alpha)$$

First calculation of self-energy in **Coulomb gauge**

He-like systems

Johan Holmberg's PhD thesis

Holmberg, Salomonson and Lindgren, Phys. Rev. A 92, 012509 (2015)

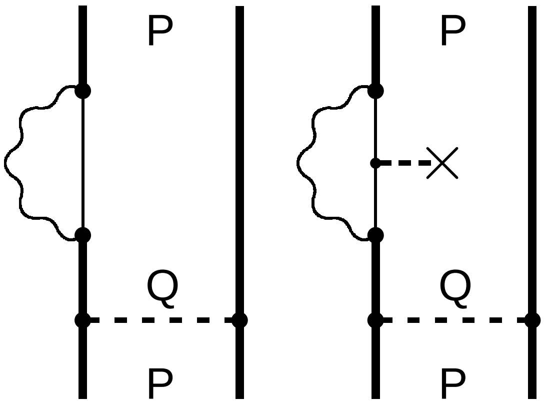


(B) and (E) are DIVERGENT

Divergence cancels due to Ward identity

He-like Argon (Z=18) Second order

Irreducible

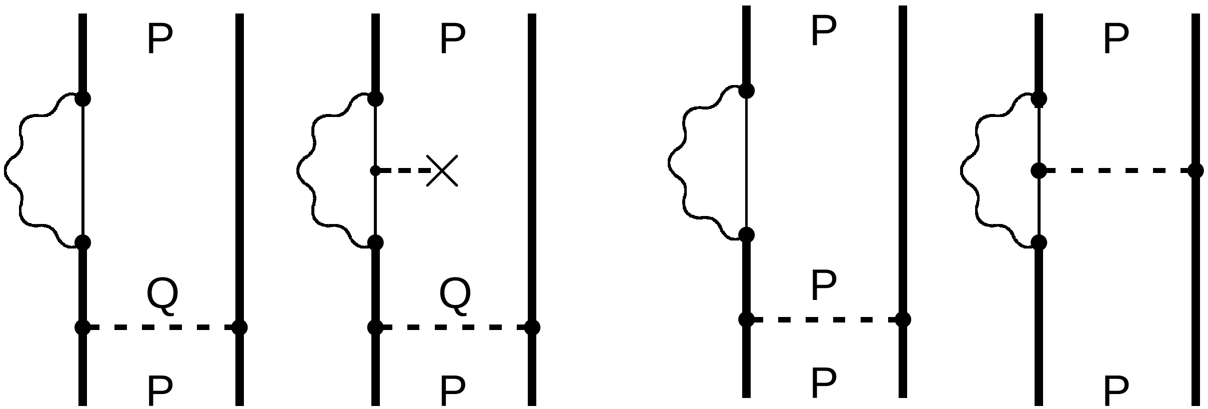


1621 meV -1707 Feynman gauge

-115.8 11.6 Coulomb gauge

He-like Argon (Z=18) Second order

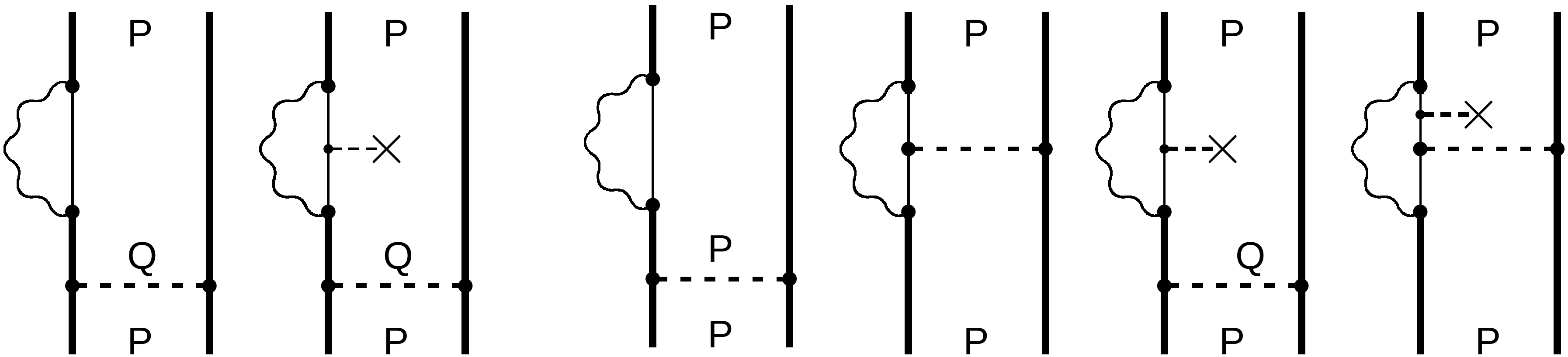
Irreducible   Model-space contr. + Vertex correction



1621 meV	-1707	3819	-3653	Feynman
-115.8	11.6	-24,8	16.2	Coulomb

He-like Argon (Z=18) Second order

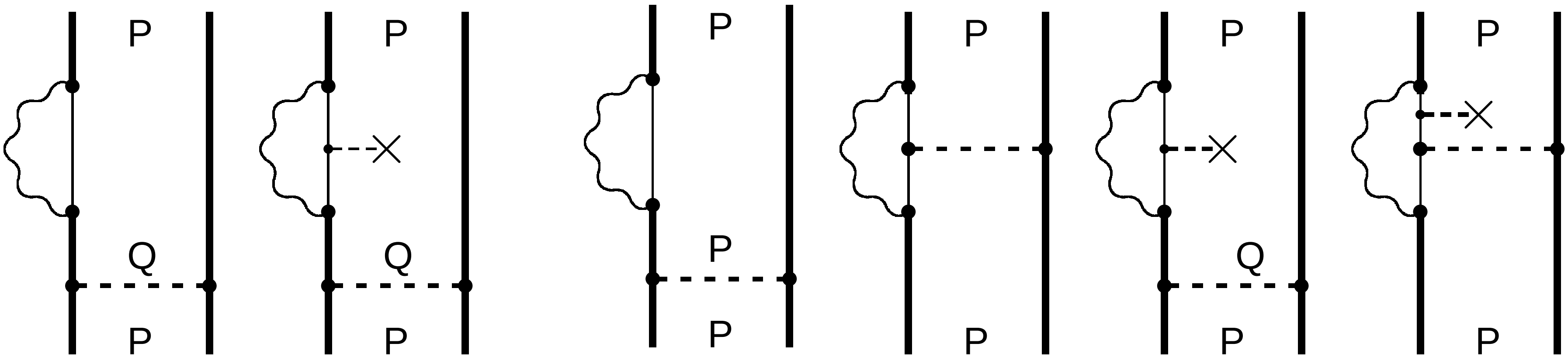
Irreducible | Model-space contr. + Vertex correction



1621 meV	-1707	3819	-3653	Feynman	-192
-115.8	11.6	-24,8	16.2	Coulomb	-1.1

He-like Argon (Z=18) Second order

Irreducible | Model-space contr. + Vertex correction



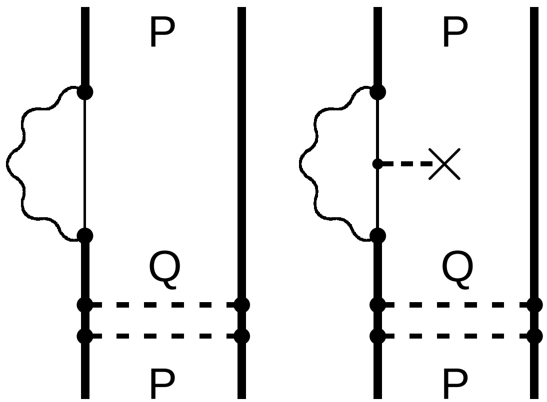
1621 meV	-1707	3819	-3653	Feynman	-192	-113
-115.8	11.6	-24,8	16.2	Coulomb	-1.1	-113.8

Gauge independe

Large cancellations in Feynman gauge

He-like Argon (Z=18) Third order

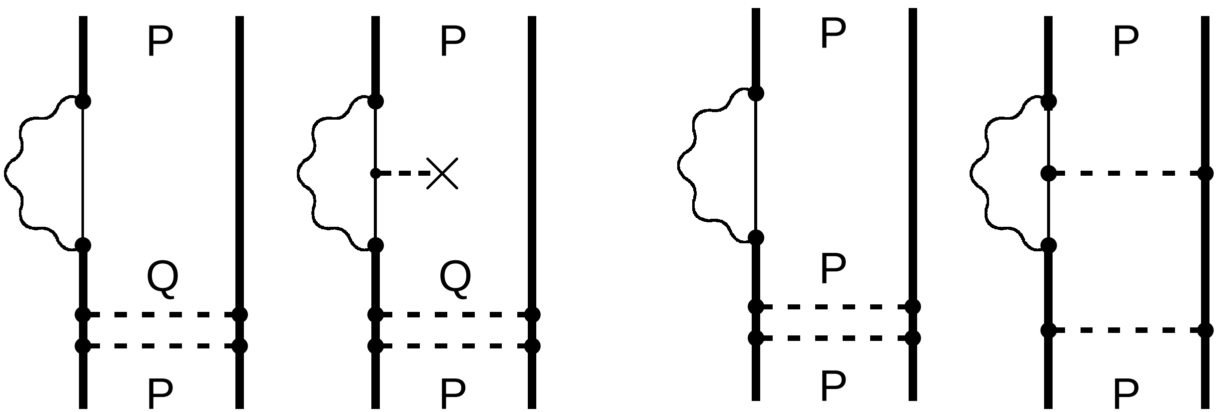
Irreducible Model-space contr. + Vertex correction



-142	71	Feynm.
4.79	-0.55	Coul.

He-like Argon (Z=18) Third order

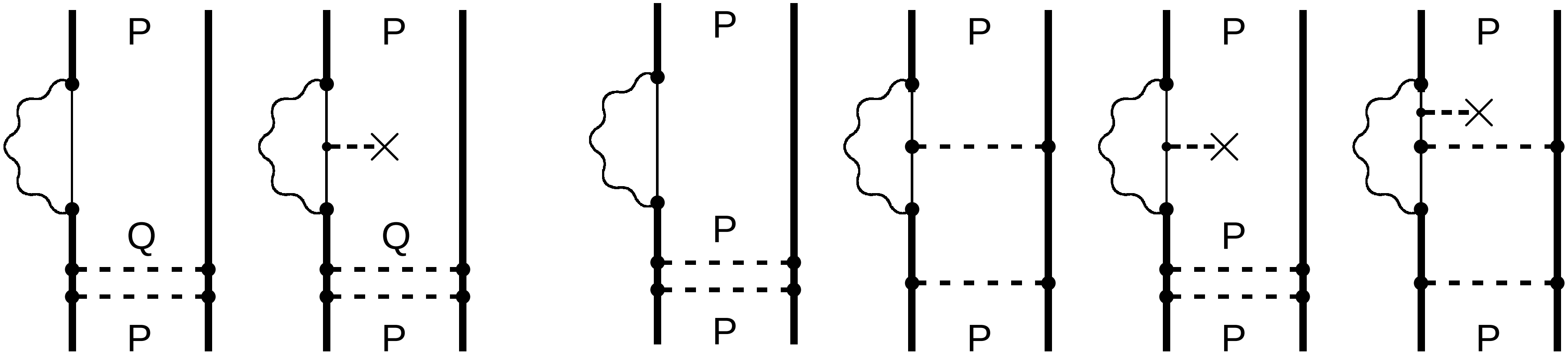
Irreducible — Model-space contr. + Vertex correction



-142	71	Feynm.	-24	54
4.79	-0.55	Coul.	1.16	-0.73

He-like Argon (Z=18) Third order

Irreducible — Model-space contr. + Vertex correction

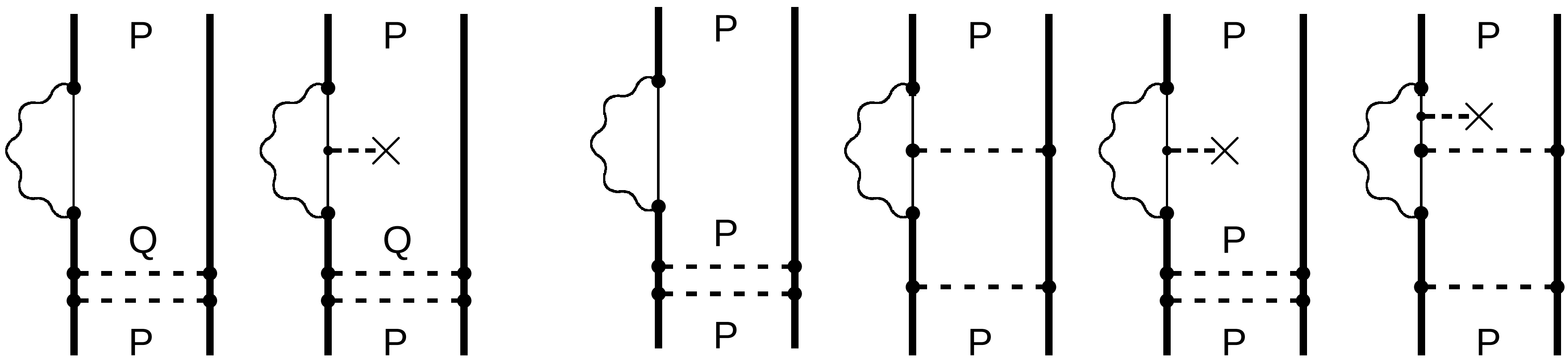


	-142	71		-24	54	???
	4.79	-0.55		1.16	-0.73	???

	Irreducible 1	Irreducible 2		Model-space 1	Model-space 2	Model-space 3–4
Feynm.	-142	71		-24	54	???
Coul.	4.79	-0.55		1.16	-0.73	???

He-like Argon (Z=18) Third order

Irreducible — Model-space contr. + Vertex correction

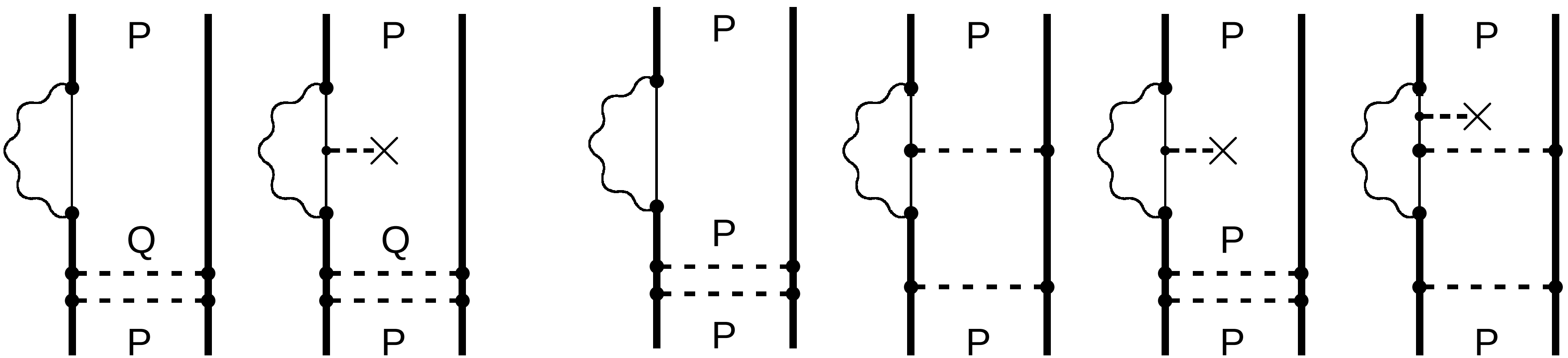


-142	71	Feynm.	-24	54	???	-41
4.79	-0.55	Coul.	1.16	-0.73	???	4.67

First calculation of radiative QED beyond second order

He-like Argon (Z=18) Third order

Irreducible   Model-space contr. + Vertex correction



-142	71	Feynm.	-24	54	???	~~−41~~
4.79	-0.55	Coul.	1.16	-0.73	???	4.67

First calculation of radiative QED beyond second order

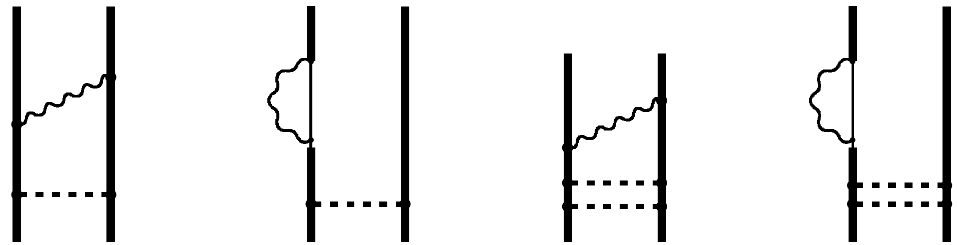
Has to be performed in **Coulomb gauge**

Holmberg, Salomonson, Lindgren, PRA 92, 012509 (2015)

Summary QED He-like gr. state

Non-radiative and radiative (in meV)

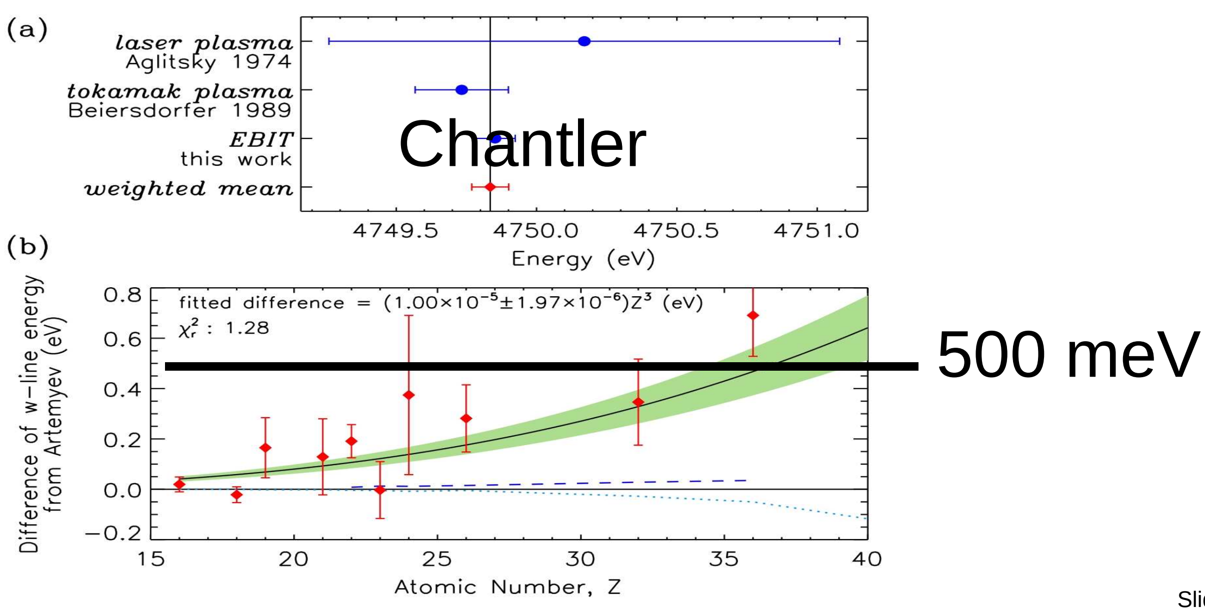
Z	Two-photon		Higher orders	
	Non-radiative	Radiative	Non-radiative	Radiative
18	4	-113	-0.8	4.7
24	10	-230	-1.2	7.0
30	21	-393	-1.5	9.6



Summary QED He-like gr. state

Higher-order QED (in meV)

Z	Holmberg 2015 (calc)	Artemyev 2005 (est'd)
14	1.6 (2)	0.8
18	2.0 (3)	0.9
24	3.9 (5)	
30	$5.6\,(8)$	-0.2
50	12 (2)	$-7.7(50)$



Summary QED He-like gr. state

Higher-order QED (in meV)

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30	$5.6\,(8)$	-0.2
50	12 (2)	$-7.7(50)$

The higher-order QED has previously been underestimated

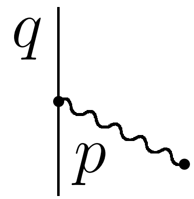
but still much too small to correspond to the Chantler discrepancies

Dynamical processes

The Green's operator can also be used in **dynamical** processes

Free particles

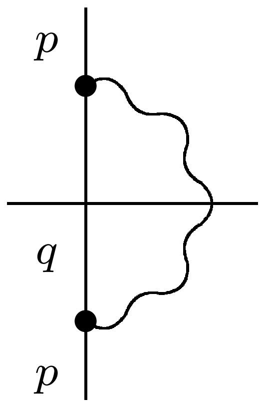
Scattering amplitude free particles



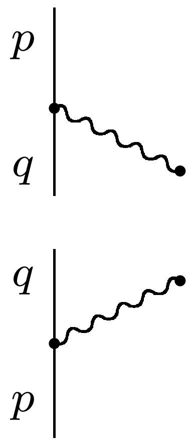
$$\langle q|S|p\rangle = 2\pi \mathrm{i}\delta(E_p - E_q)\,\tau(p\to q)$$

Optical theorem for free particles

$$-2Im\langle p|\mathrm{i}S|p\rangle = \sum_q \left|2\pi\delta(E_p - E_q)\tau(p\to q)\right]^2$$



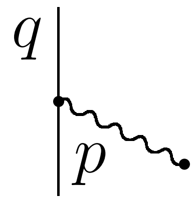
Forward scattering



Cross section

Free particles

Scattering amplitude free particles



$$\langle q|S|p\rangle = 2\pi \mathrm{i}\delta(E_p - E_q)\,\tau(p \to q)$$

Optical theorem for free particles

$$-2Im\langle p|\mathrm{i}S|p\rangle = \sum_q \Big|2\pi\delta(E_p - E_q)\tau(p \to q)\Big]^2$$

The imaginary part of the forward scattering amplitude is proportional to the total cross section

Bound particles

$$S = U(\infty, -\infty) = U_{\rm Cov}(\infty, -\infty)$$

S-matrix becomes singular for bound states with intermediate model-space states

Optical theorem for bound particles

$$-2Im\langle p|\mathrm{i}\,\mathcal{G}(\infty, -\infty)|p\rangle = \sum_q \Big|2\pi\delta(E_p - E_q)\tau(P \to q)\Big]^2$$

$\mathcal{G}(\infty, -\infty)$ is identical to the S-matrix, if there are no intermediate model-space states

$\mathcal{G}$ always regular: "S-matrix cleaned from singularities"

Bound particles

$$P\,\mathrm{i}\,\mathcal{G}(\infty,-\infty) = 2\pi\delta(E_{\mathrm{in}} - E_{\mathrm{out}})\,W$$

$$-2Im\langle p|\mathrm{i}\mathcal{G}(\infty,-\infty)|p\rangle = \sum_q \left|2\pi\delta(E_p - E_q)\tau(p\to q)\right]^2$$

$$-2Im\langle p|W|p\rangle = \sum_q 2\pi\delta(E_p - E_q)\tau(p\to q)^2$$

$$P\,\mathrm{i}\,\mathcal{G}(\infty,-\infty) = 2\pi\delta(E_{\mathrm{in}} - E_{\mathrm{out}})\,W$$

$$-2Im\langle p|\mathrm{i}\mathcal{G}(\infty,-\infty)|p\rangle = \sum_q \Big|2\pi\delta(E_p - E_q)\tau(p \to q)\Big]^2$$

$$\boxed{-2Im\langle p|H_{\mathrm{eff}}|p\rangle = \sum_q 2\pi\delta(E_p - E_q)\tau(p \to q)^2}$$

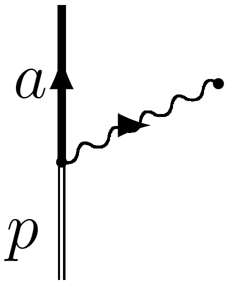
$$H_{\mathrm{eff}} = PH_0P + W$$

Optical theorem for **free and bound** particles

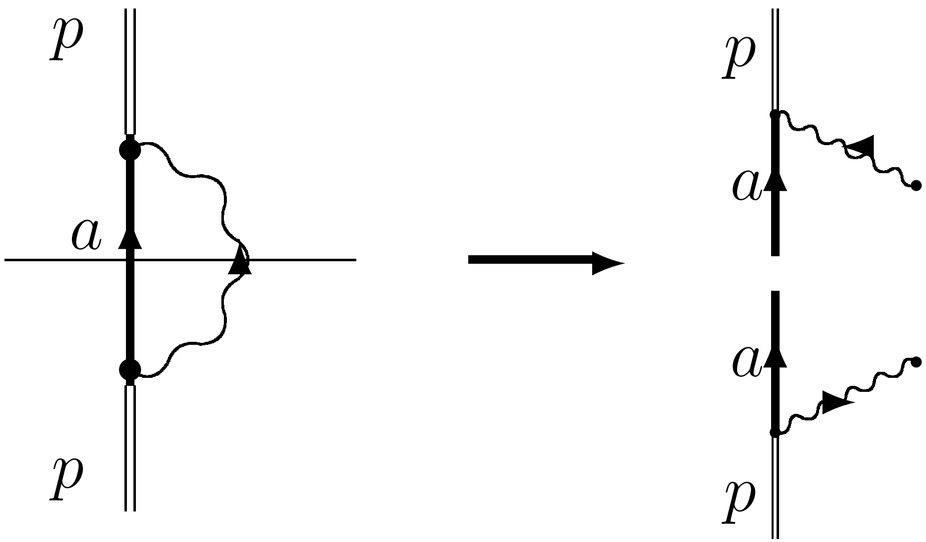
Lindgren, Salomonson, Holmberg, PRA **89**, 062504 (2014)

Radiative recombination

Lindgren, Salomonson, Holmberg, PRA **89**, 062504 (2014)
Shabaev *et al,* PRA **61**, 052112 (2000)



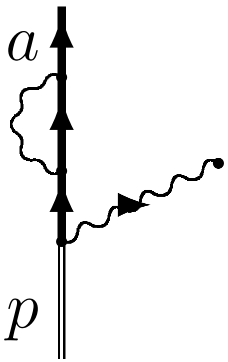
First-order amplitude



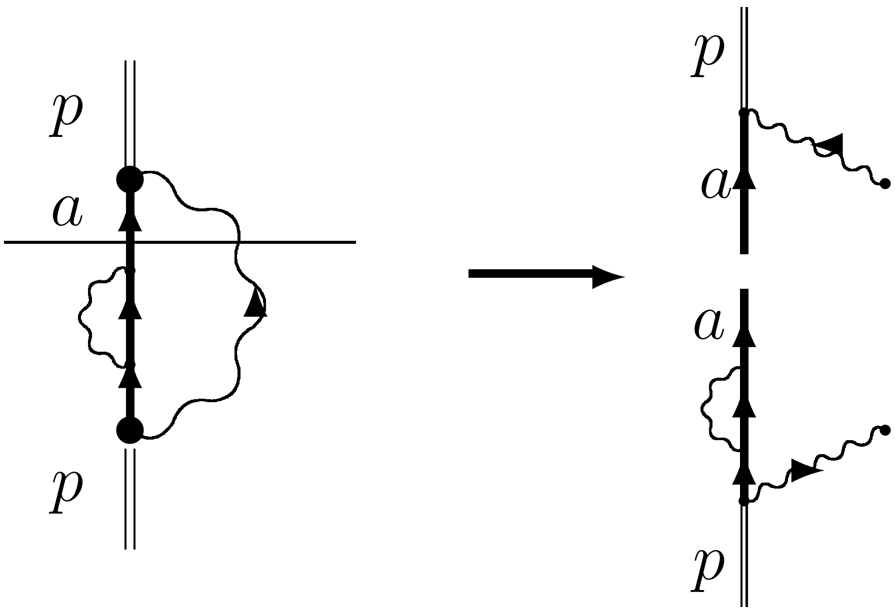
Forward scattering   Cross section

Radiative recombination

Self-energy insertion



First-order amplitude



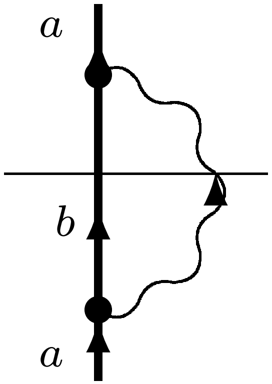
Forward scattering   Cross section

Radiative recombination

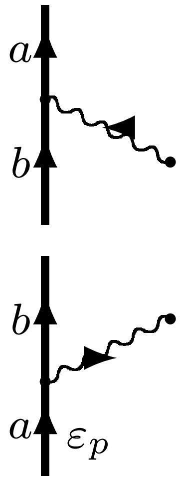
Self-energy insertion leads to singularity

that is taken care of in the **Green's operator**.

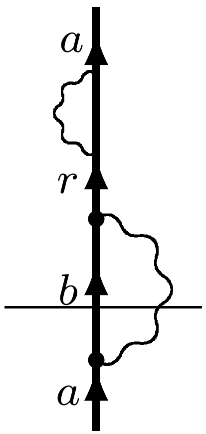
Radiative decay

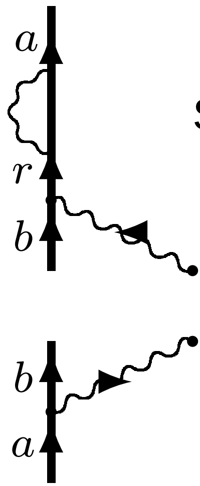


Forward scattering



Cross section





Self-energy insertion (MSC)

Radiative decay

$1s - 2p_{1/2}$ transition in H-like Uranium

Magnetic quadrupole to electrical dipole ampitude ratio

	M2/E1
Dirac	0.084229
QED	0.000197

Expt't: Stöhlker et al. PRL **105**, 243002 (2010)
JPB 48,144031 (2015)

Theory: Holmberg, Artemyev, Surzhykov, Yerohkin, Stöhlker, SSPRA 92, 042510 (2015)

Conclusions and Outlook

The **Green's operator** is a
time-dependent wave operator

Can combine **time-dependent** and **time-independent** perturbations, **unifying QED and MBPT**

Can be used for **stationary** as well as **dynamical** problems (**real** and **imaginary** parts, respectively)

Improves the accuracy of theoretical estimates one order of magnitude

Conclusions and Outlook

The **Green's operator**

has been used to evaluate **QED beyond second order**, employing **Coulomb gauge** for radiative QED

applied to **dynamical problems** to derive

the **Optical Theorem** for bound systems

to evaluate the QED effect in **radiative recombination** and in **radiative decay** (together with GSI, Jena)

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The Humboldt Foundation

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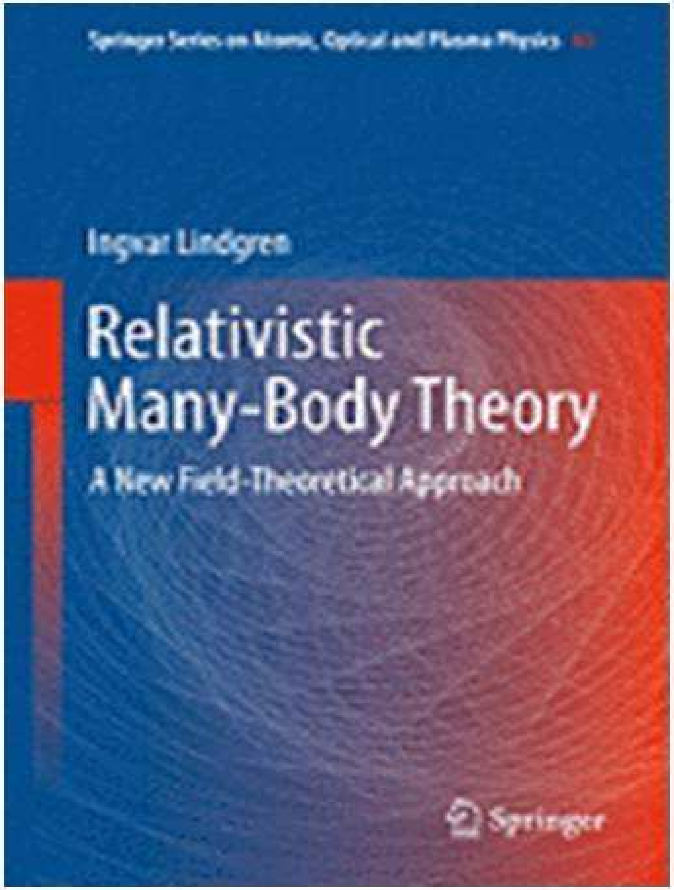
Gesellschaft für Schwerionenforschung

Thank you!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