Combined Many-Body-QED Calculations

Numerical solution of the Bethe-Salpeter equation

Ingvar Lindgren, Sten Salomonson, and Daniel Hedendahl
Department of Physics, Göteborg University

Symposium in Memory of Gerhard Soff

Frankfurt, April 2005

Bound/SoffSymp

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Einstein Centennial paper: Can. J. Physics, March 2005

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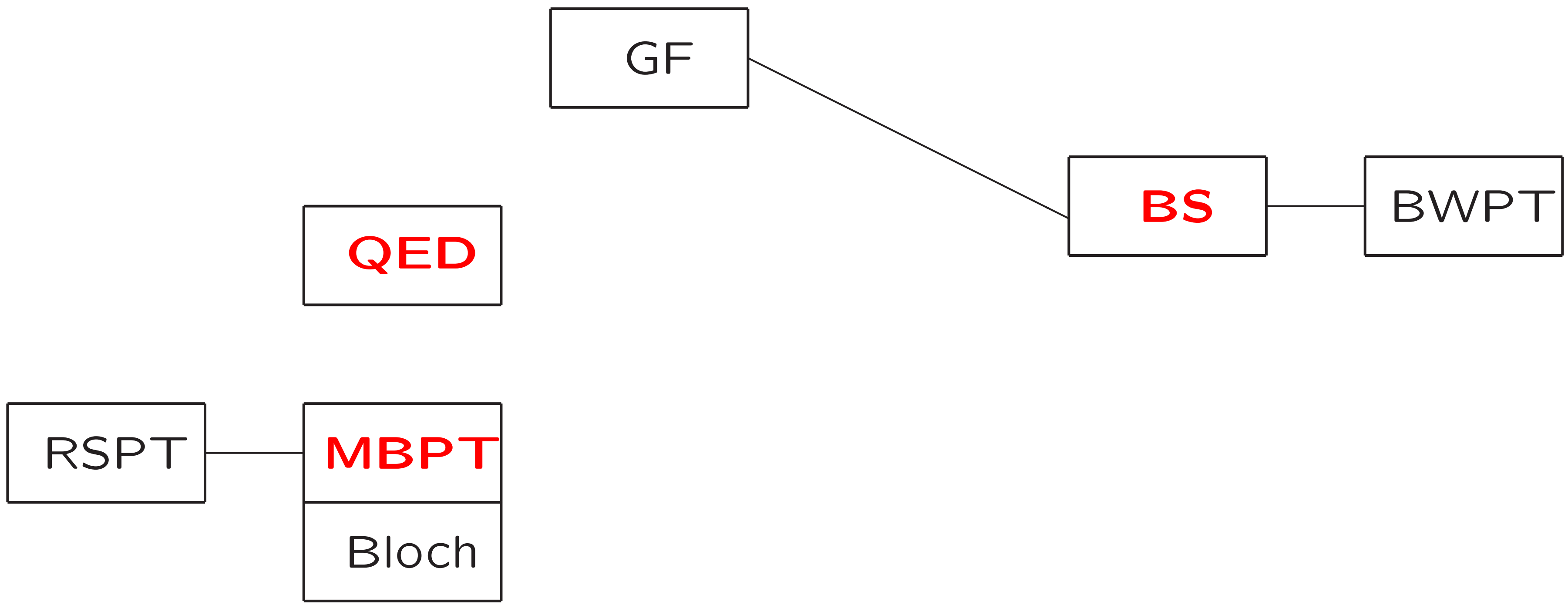
MBPT–QED–Bethe-Salpeter

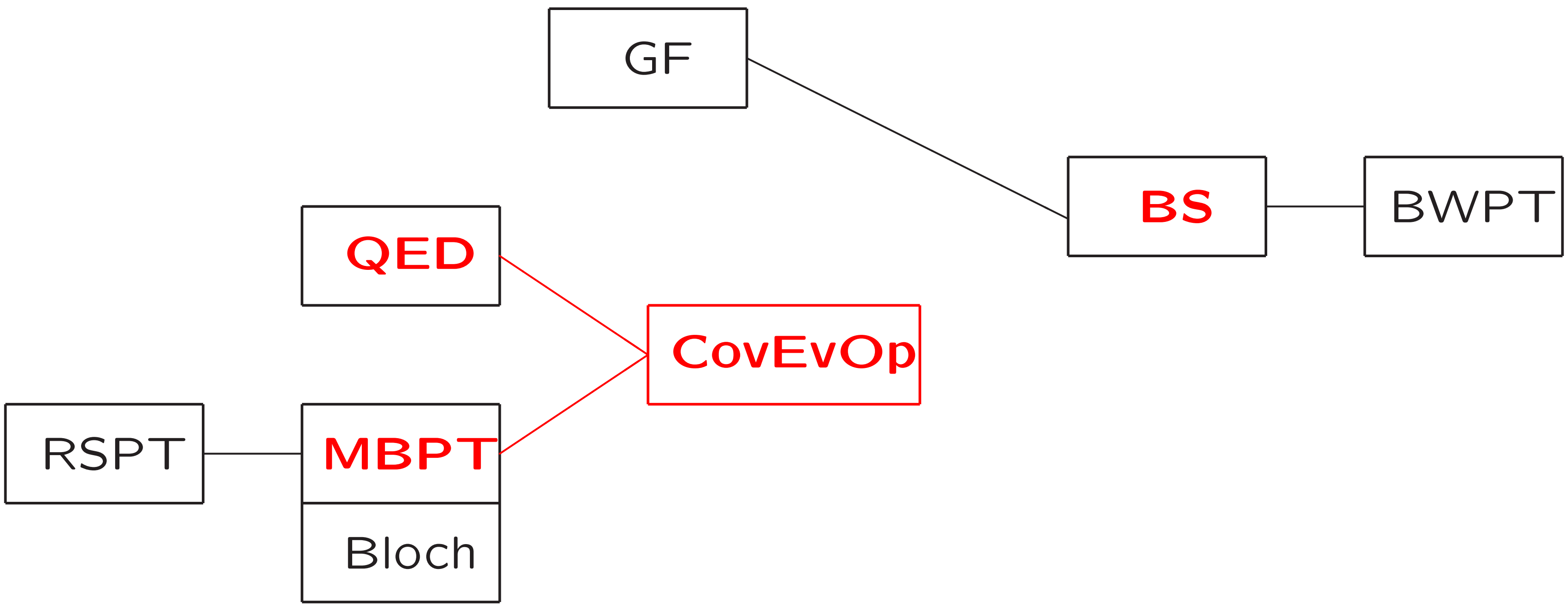
Normally regarded as separate techniques



MBPT–QED–Bethe-Salpeter

MBPT and QED combined in CovEvOp

Physics Reports **389**, 161 (2004)



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CovEvOp can connect to the BS eqn

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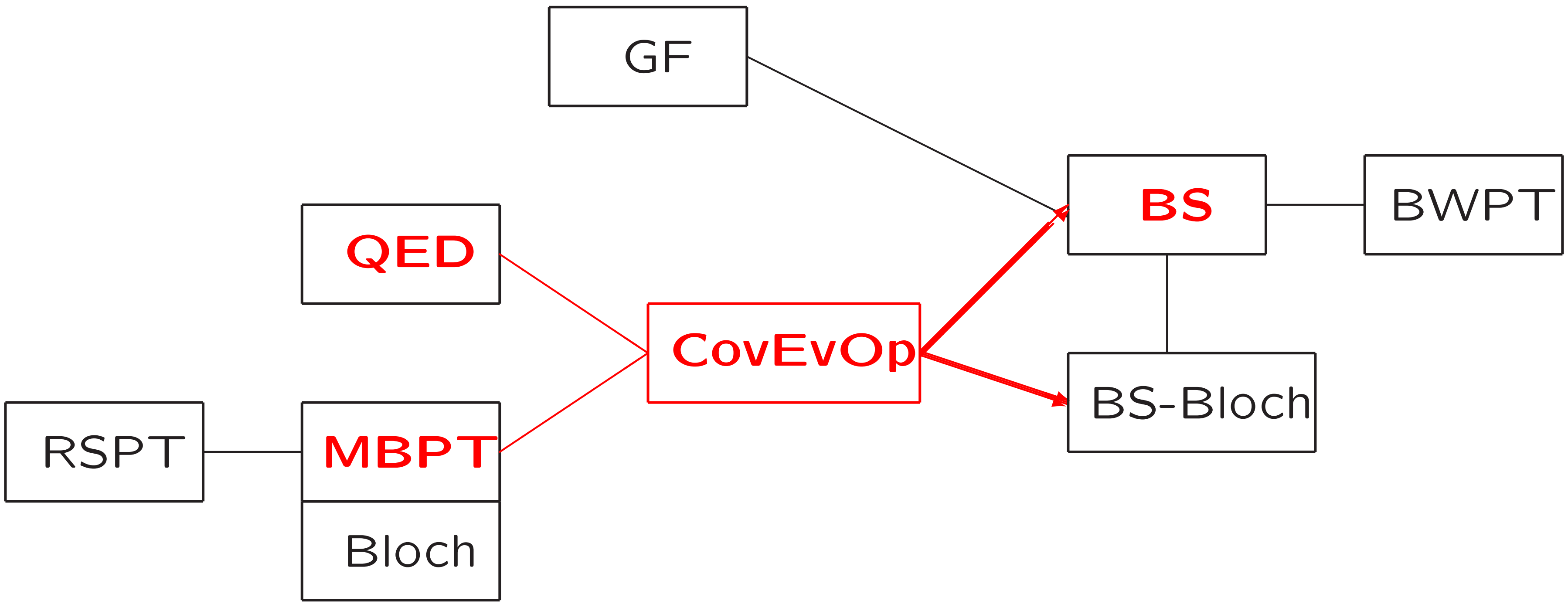

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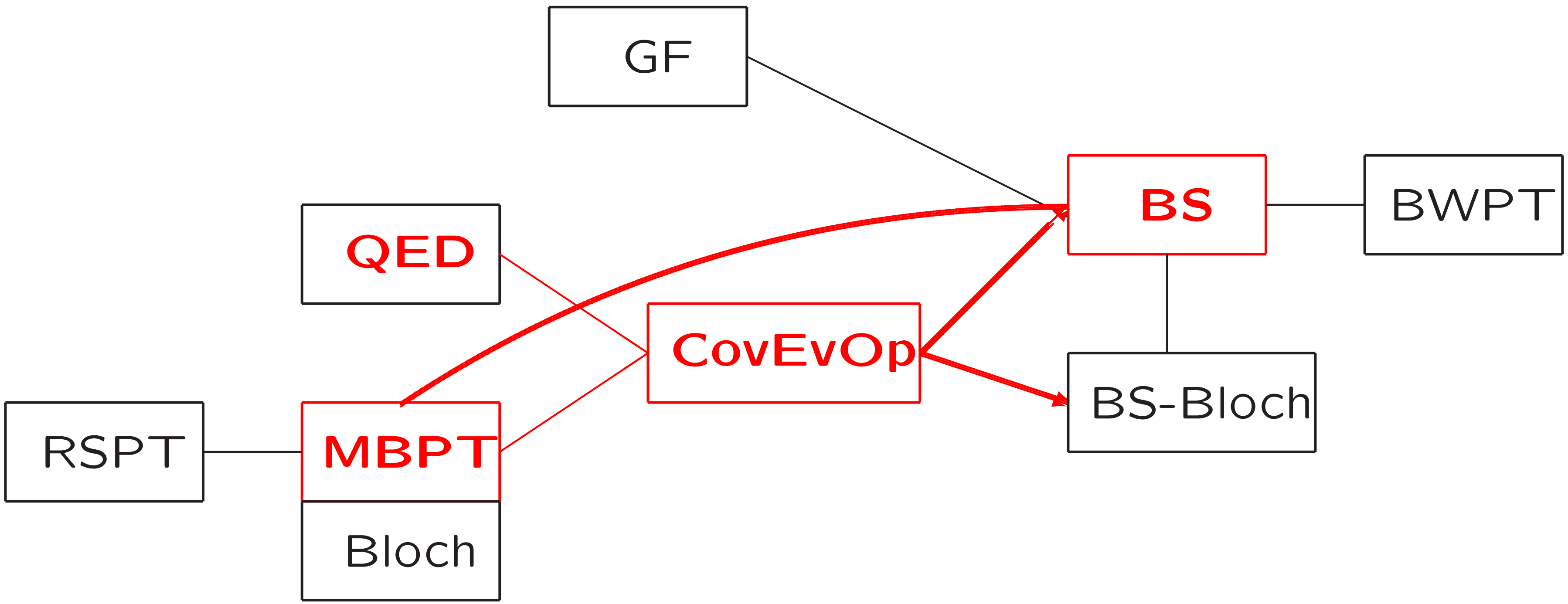
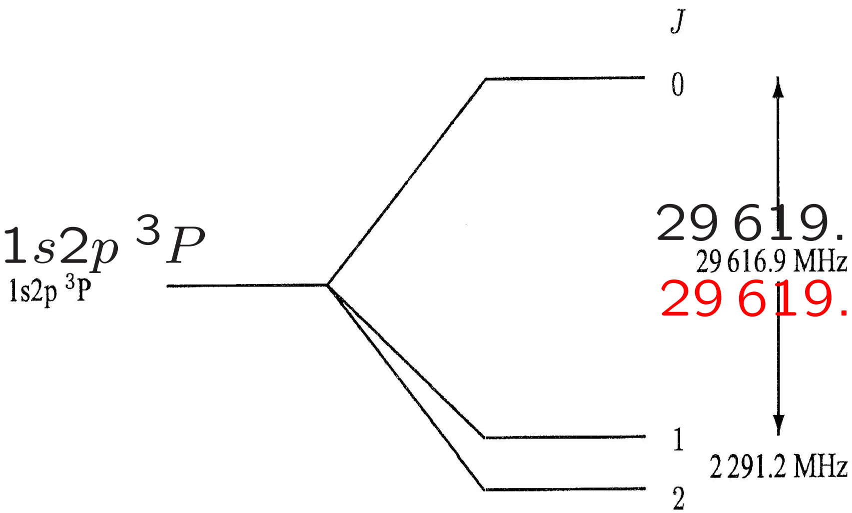


Connects MBPT and full BS eqn

Fine structure of helium atom

$1s2p\ ^3P$

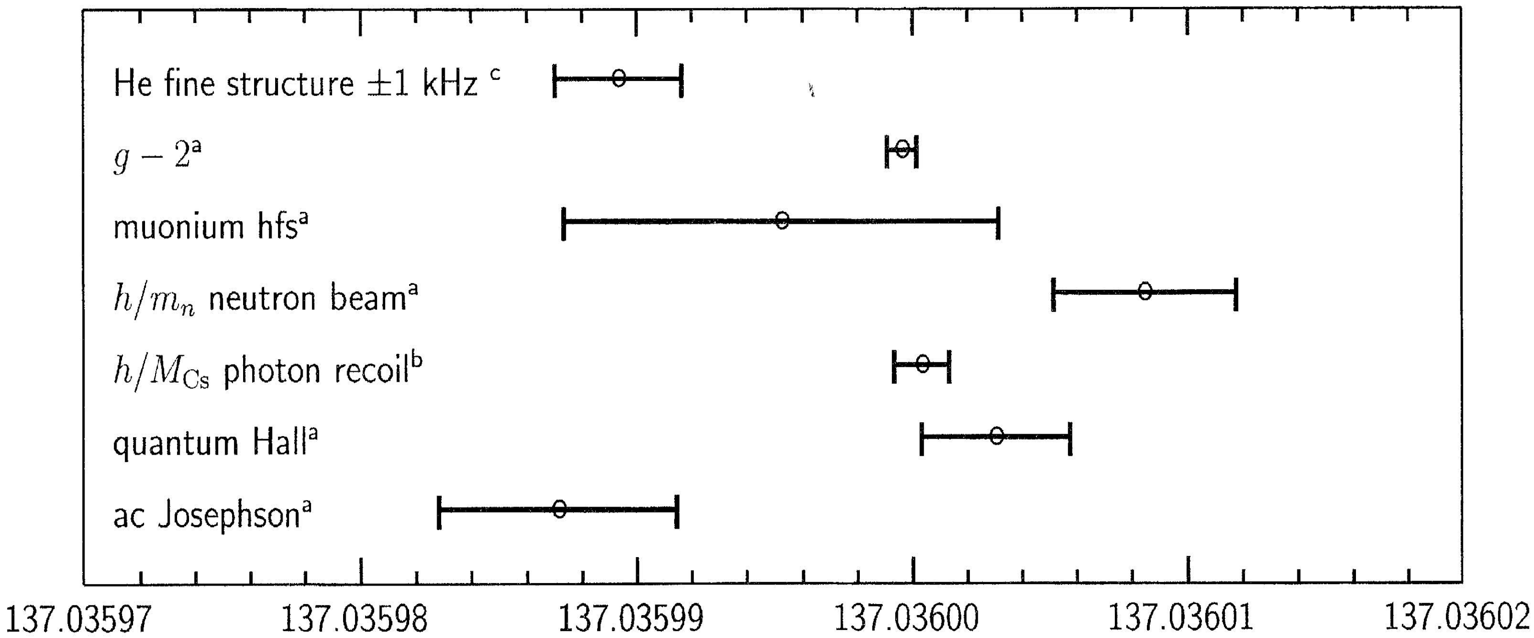


29 619.9509(9) MHz

29 619.9464(2) Theory

Fine-structure constant

(from Drake, Can. J. Phys. **80**, 1195 (2002))



Standard approaches for QED calculations

1. Analytical

α, $Z\alpha$ expansions from **Bethe-Salpeter** eqn
Evaluated with **correlated** wave function
Applicable to **light** elements
(Drake, Pachucki and others)

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S-matrix, **Green's function**

QED effects evaluated **numerically** with **uncorrelated** wave functions

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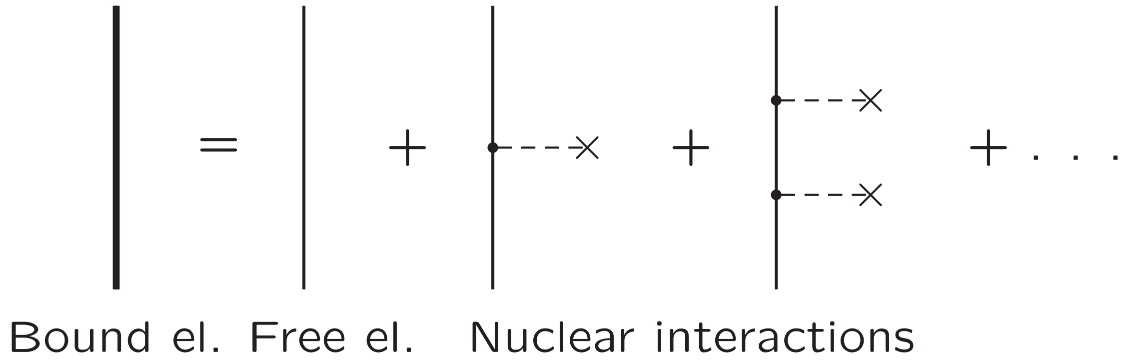
Relativistic Furry picture, **only α expansion**

Numerical approach

1. **Start from hydrogenic Dirac orbitals (Green's functions) in nuclear potential (Furry picture)**



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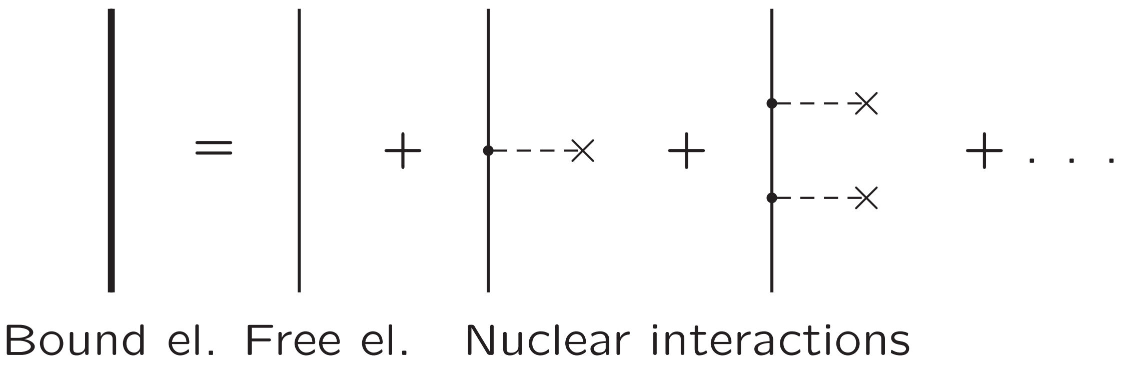
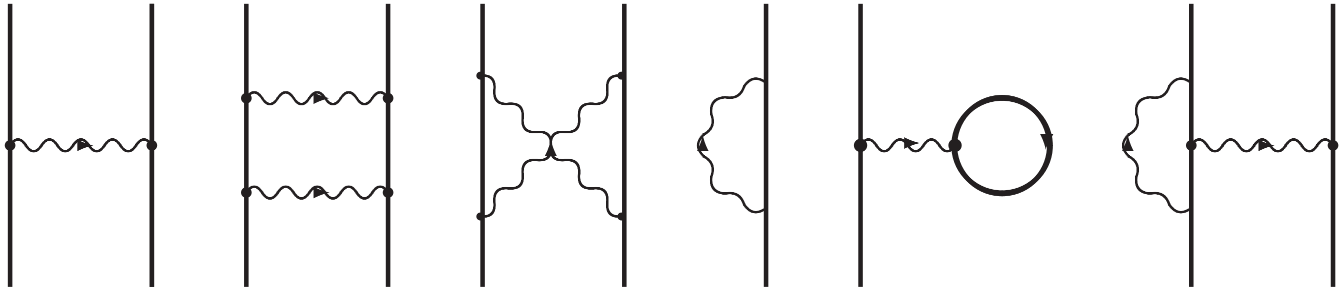


All orders in $Z\alpha$

2. Evaluate one-, two-, ... photon exchange



Non-radiative **Radiative**

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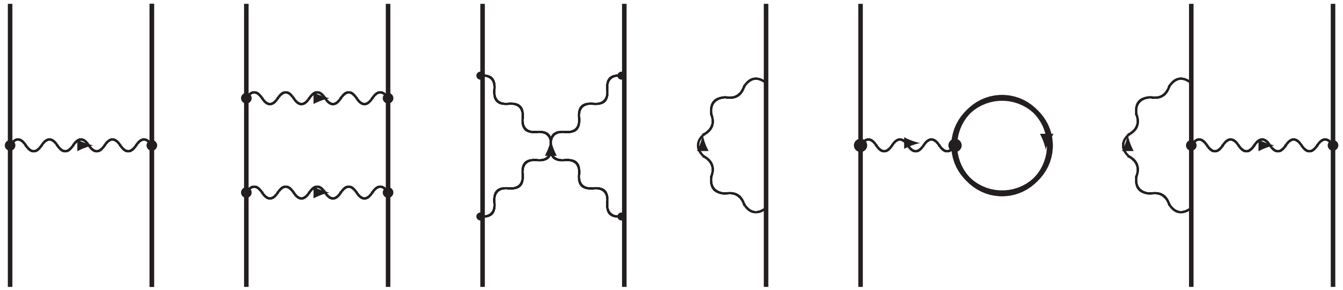

Non-radiative Radiative

Applied mainly to heavy elements

Only one- and two-photon exchange can be evaluated

Electron correlation poorly treated

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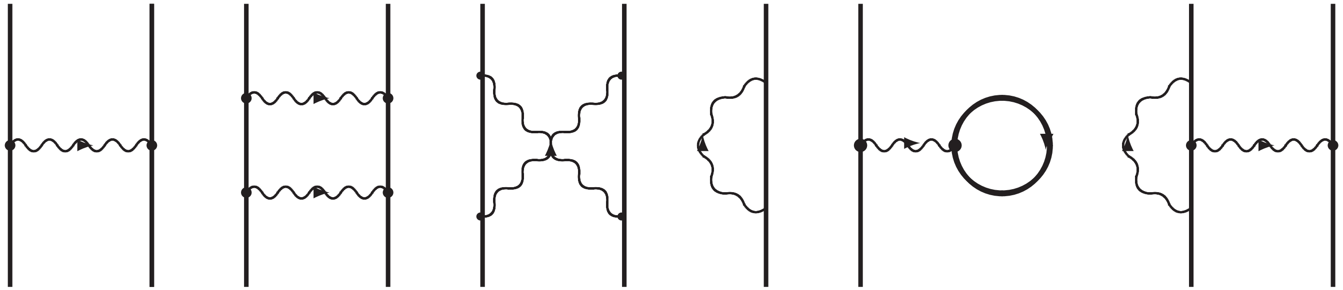

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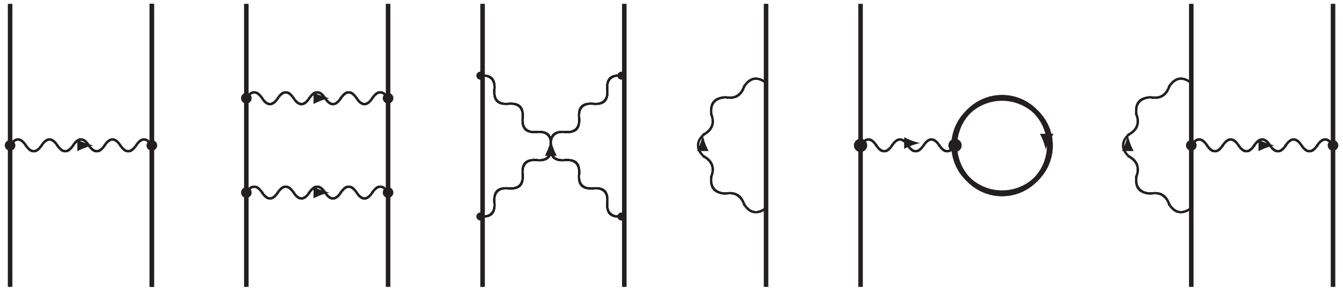

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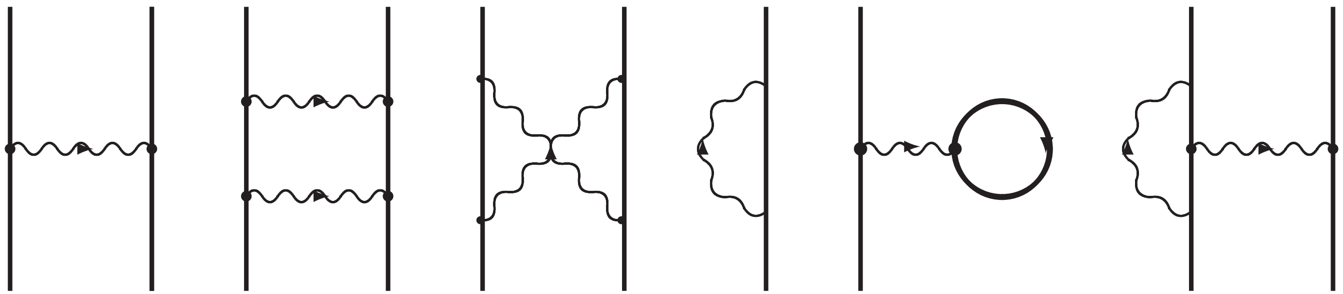

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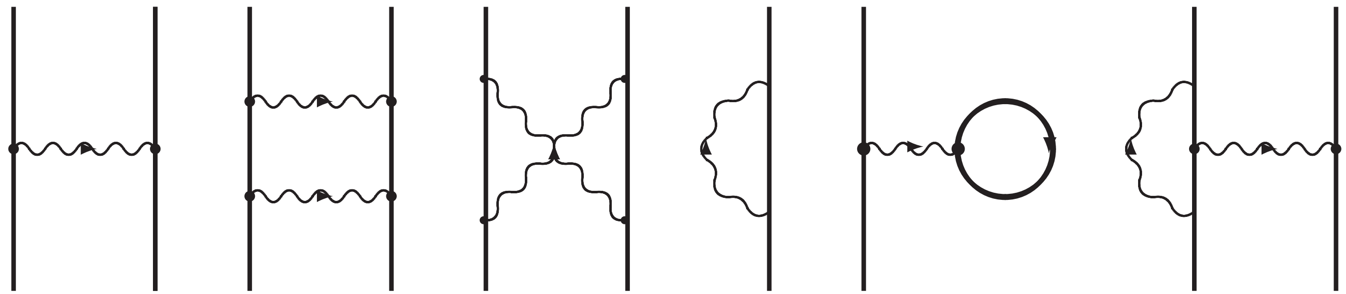

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Can the advantages of the

analytical and numerical approaches

be combined?

Standard MBPT

1. **Model space** (P)

Strongly mixed states included in the model space
Important for **quasi-degeneracy** (fine structure).

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Ω evaluated by perturbation expansion from **Bloch eqn**

$$\big[\Omega, H_0\big] P = \big(V\,\Omega - \Omega\, P V \Omega\big) P \qquad (V = 1/r_{12})$$

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The Bloch eqn can handle quasi-degeneracy

The Bloch eqn can also be used to generate

All-order MBPT procedures

Coupled-Cluster Approach

$$\Omega = \{e^S\} \qquad S = S_1 + S_2 + \cdots$$

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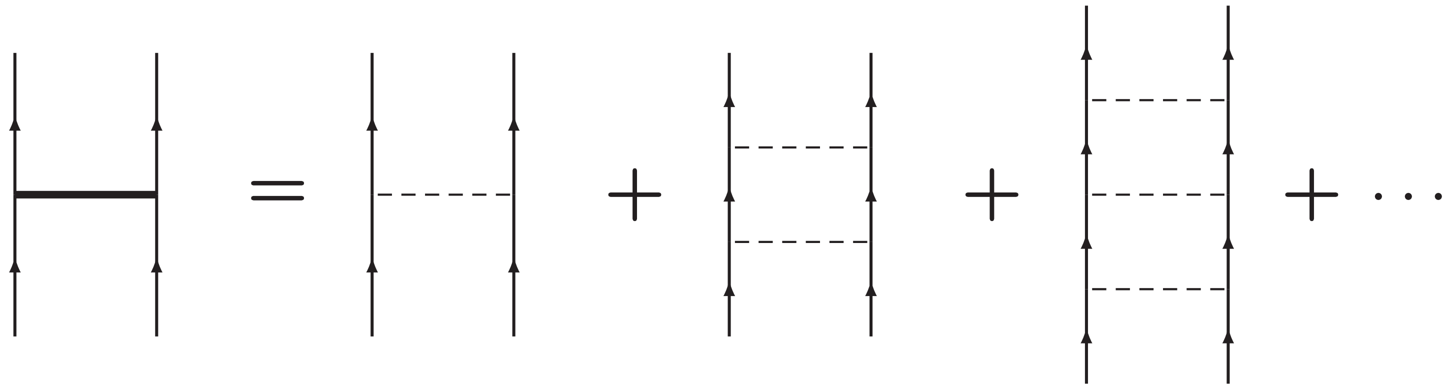
Pair function (S_2)



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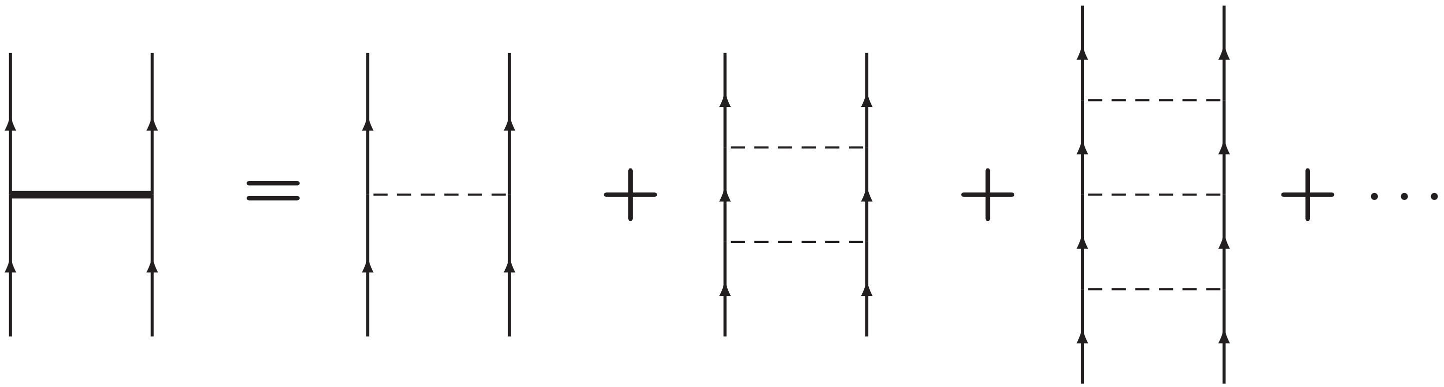

(Pair) correlation can be treated to all orders

The MBPT technique can handle

quasi-degeneracy

and correlation effects to all orders.

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and correlation effects to all orders.

Can these effects be incorporated into a

numerical QED procedure?

Time-dependent perturbation theory

Time-evolution operator:

$$\Psi(t) = \boldsymbol{U(t, t_0)}\Psi(t_0)$$

$$\boldsymbol{U(t, t_0)} = 1 + \sum_{n=1}^{\infty} \frac{(-\mathrm{i})^n}{n!} \int_{t_0}^{t} \mathrm{d}^4 x_n \ldots \int_{t_0}^{t} \mathrm{d}^4 x_1 \, T_{\mathrm{D}}\Big[\mathcal{H}'_{\mathrm{I}}(x_n) \ldots \mathcal{H}'_{\mathrm{I}}(x_1)\Big]$$

$\mathcal{H}'_{\mathrm{I}}(x)$ the perturbation density in Interaction Picture

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$\mathcal{H}'_{\mathrm{I}}(x)$ the perturbation density in Interaction Picture

Adiabatic damping:

$$\mathcal{H}'_{\mathrm{I}}(x) \Rightarrow \mathcal{H}'_{\mathrm{I}}(x)\, e^{-\gamma|t|} \qquad \boldsymbol{U(t, t_0)} \Rightarrow \boldsymbol{U_\gamma(t, t_0)} \qquad \Psi(t) \to \Psi_\gamma(t)$$

$$\Psi_0 = \lim_{t \to -\infty} \Psi_\gamma(t)$$

$\boldsymbol{U(\infty, -\infty) = S}$ is the $\boldsymbol{S - matrix}$

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but we shall consider **finite** final times:

$$U(t, -\infty)$$

Gell-Mann–Low theorem

Time-independent wave function given by

$$\boldsymbol{\Psi} = \lim_{\gamma \to 0} \frac{\boldsymbol{U_\gamma(0,-\infty)}\big|\boldsymbol{\Psi_0}\big\rangle}{\langle \boldsymbol{\Psi_0}|\boldsymbol{U_\gamma(0,-\infty)}\,|\boldsymbol{\Psi_0}\rangle}$$

$\big|\boldsymbol{\Psi_0}\rangle = \boldsymbol{P\Psi}$ unperturbed wave function

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The evolution operator **singular** as $\gamma \to 0$

The denominator cancels the singularities

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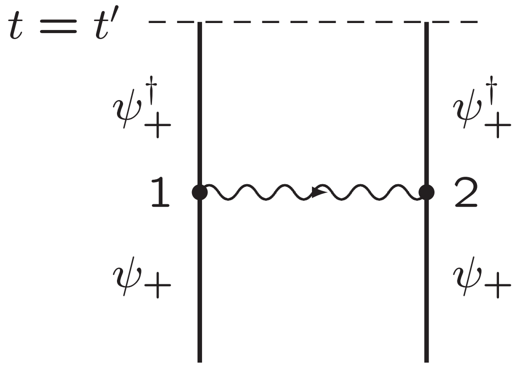
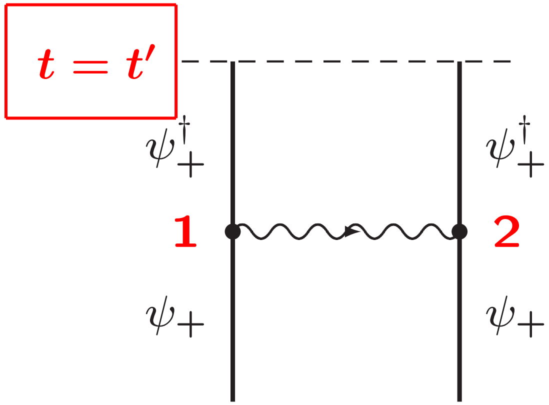
Brueckner-Goldstone Linked-Diagram Theorem

Evolution operator for single-photon exchange



$$U^{(2)}(t', -\infty) = -\frac{1}{2}\iint_{-\infty}^{t'} \mathrm{d}^4x_1\,\mathrm{d}^4x_2\,\psi_+^\dagger(x_1')\psi_+^\dagger(x_2')\,\alpha_1^\mu\,\mathrm{i}\,\underbrace{D_{\mathrm{F}\mu\nu}(x_1 - x_2)}_{\text{Photon propagator}}\,\alpha_2^\nu\,\psi_+(x_2)\,\psi_+(x_1)\,\mathrm{e}^{-\gamma(|t_1|+|t_2|)}$$

Evolution operator for single-photon exchange



$$U^{(2)}(t', -\infty) = -\frac{1}{2} \iint_{-\infty}^{t'} \mathrm{d}^4 x_1\, \mathrm{d}^4 x_2\, \psi_+^\dagger(x_1')\psi_+^\dagger(x_2')\, \alpha_1^\mu\, \mathrm{i}\, \underbrace{D_{\mathrm{F}\mu\nu}(\boldsymbol{x}_1 - \boldsymbol{x}_2)}_{\text{Photon propagator}}\, \alpha_2^\nu\, \psi_+(x_2)\, \psi_+(x_1)\, \mathrm{e}^{-\gamma(|t_1|+|t_2|)}$$

t_1 and t_2 integrated only from $-\infty$ to t'.

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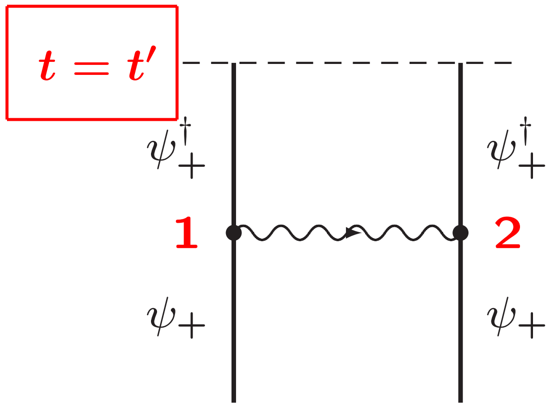

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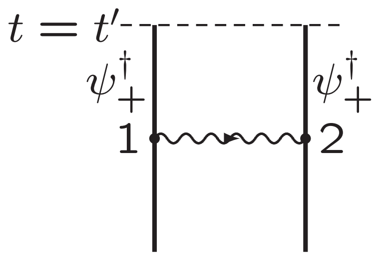
Non-covariant

Covariant evolution operator

Physics Reports **389**, 161 (2004); Phys. Rev. A **64**, 062505 (2001)



Particle states out

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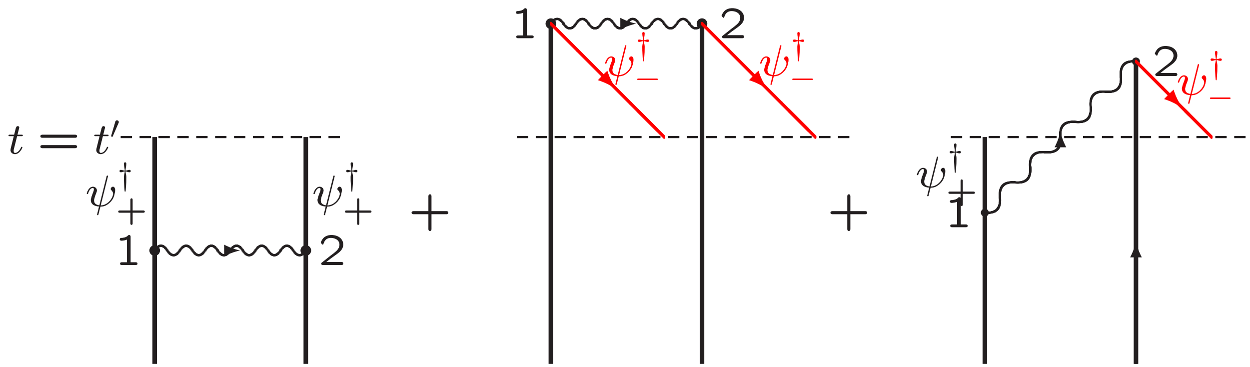

Particle states out
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Hole states out

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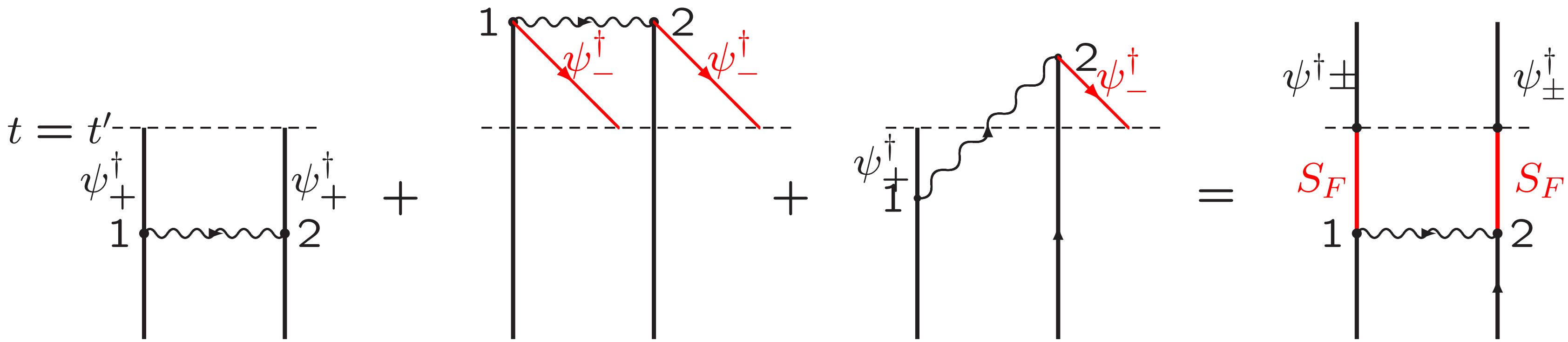

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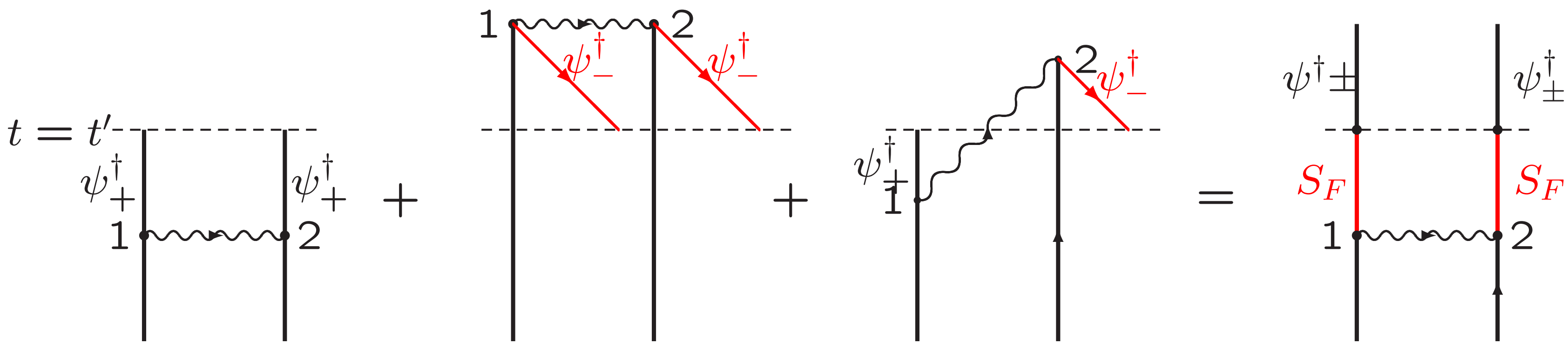

Particle states out
Non-covariant

Hole states out

El. propagators out
Covariant

$$U^{(2)}_{\rm Cov}(t', -\infty) = -\frac{1}{2}\iint \mathrm{d}^3\boldsymbol{x}'_1 \mathrm{d}^3\boldsymbol{x}'_2\, \psi^\dagger(x'_1)\psi^\dagger(x'_2) \iint_{-\infty}^{\infty} \mathrm{d}^4x_1\, \mathrm{d}^4x_2$$
$$\times \quad \mathrm{i}S_{\rm F}(x'_1, x_1)\, \mathrm{i}S_{\rm F}(x'_2, x_2)\, \alpha_1^\mu\, \mathrm{i}D_{\mathrm{F}\mu\nu}(x_2 - x_1)\, \alpha_2^\nu\, \psi(x_2)\, \psi(x_1)\, \mathrm{e}^{-\gamma(|t_1|+|t_2|)}$$

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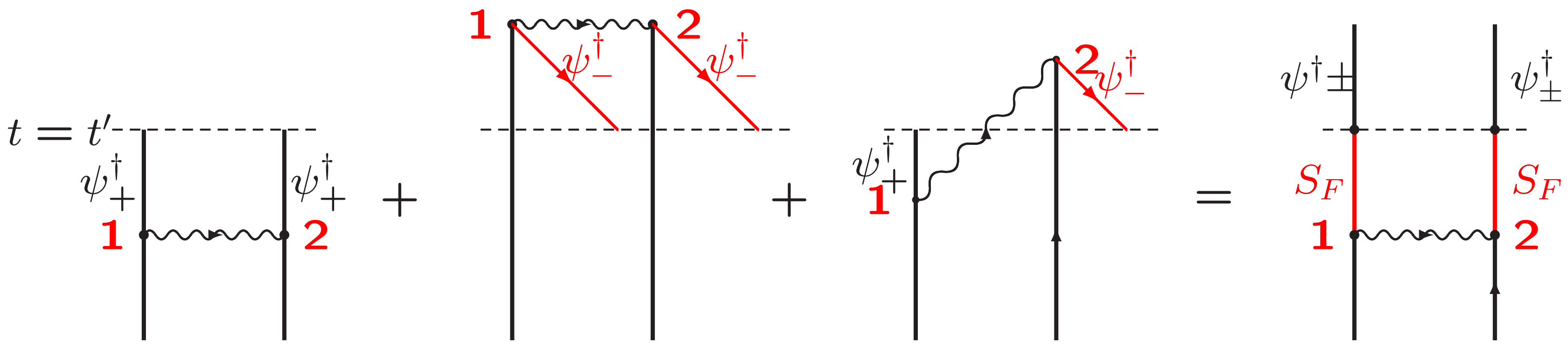

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t_1 and t_2 integrated over all times

The evolution operator is singular

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Reduced evolution operator is regular

$$U_\gamma(t,-\infty)P = P + \boxed{\widetilde{U}_\gamma(t,-\infty)}\; P\, U_\gamma(0,-\infty)P$$

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Factorization theorem for $t = 0$:

$$U_\gamma(0,-\infty)P = \underbrace{\left[1 + Q\,\widetilde{U}_\gamma(0,-\infty)\right]}_{\text{Regular}}\ \underbrace{P\,U_\gamma(0,-\infty)}_{\text{Singular}}\,P$$

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Wave operator Ω

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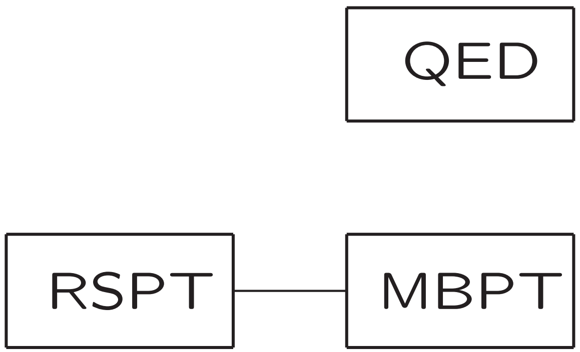
Links with MBPT

MBPT and QED



MBPT and QED combined in Cov.Ev.Op. method

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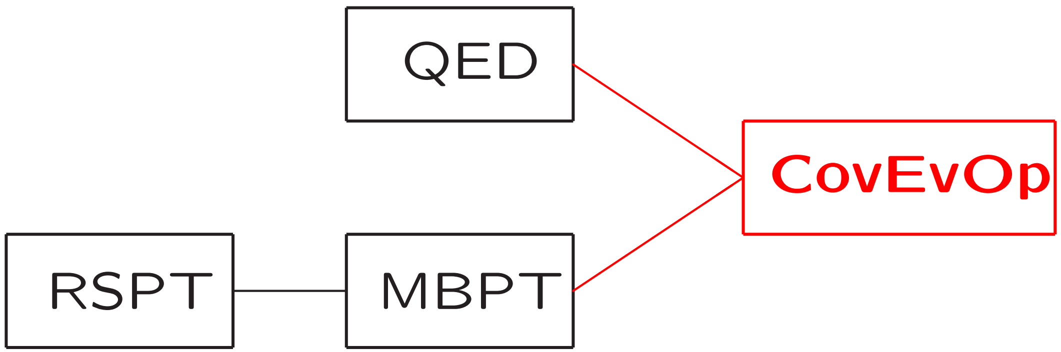
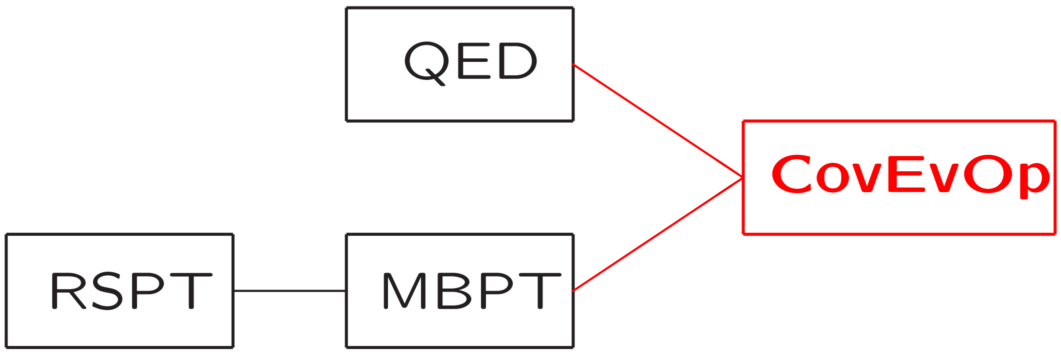


MBPT and QED

combined in Cov.Ev.Op. method

Physics Reports **389**, 161 (2004)

Can handle quasi-degeneracy



Fine structure of He-like ions

—

Z	$^3P_1 - ^3P_0$	$^3P_2 - ^3P_0$	$^3P_2 - ^3P_1$	
2	29616.9509(9)		2291.1759(10) MHz	Expt'l
	29616.9496(10)		2291.1736(11)	Theory
3	155704.27(66)		-62678.41(66) MHz	Expt'l
	155703.4(1,5)		-62679.4(5)	Drake
9	701(10)		4364,517(6) μH	Expt'l
	680	5050	4362(5)	Drake
	690	5050	4364	Plante
	690	**5050**		**Present**
10	1371(7)	8458(2) μH		Expt'l
	1361(6)	8455(6)	265880	Drake
	1370	8469	265860	Plante
	1370	**8460**		**Present**
18		124960(30) μH		Expt'l
		124810(60)		Drake
		124942		Plante
		124940		**Present**

I. Lindgren, S. Salomonson, and B. Åsén, Physics Reports **389**, 161 (2004)
I. Lindgren, B. Åsén, S. Salomonson, and A.-M. Pendrill, PRA **64**, 062505 (2001)

Fine structure of He-like ions

$$^3P_1 = \frac{1}{\sqrt{2}}[\langle 1s, 2p_{1/2}| + \langle 1s, 2p_{3/2}|]$$ **quasi-degenerate**

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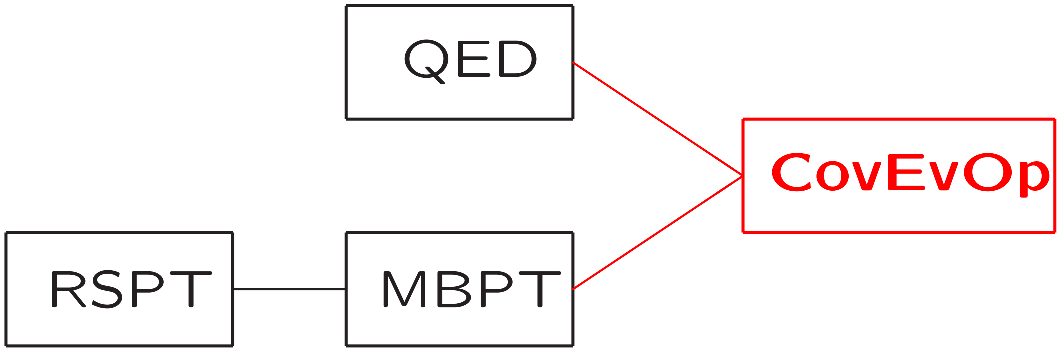
MBPT and QED

Quasi-degeneracy with Cov.Ev.Op. method



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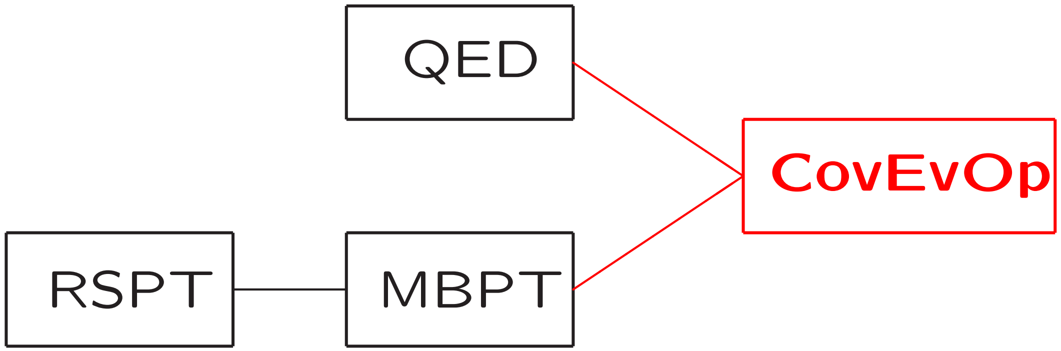
QED with correlated wave functions



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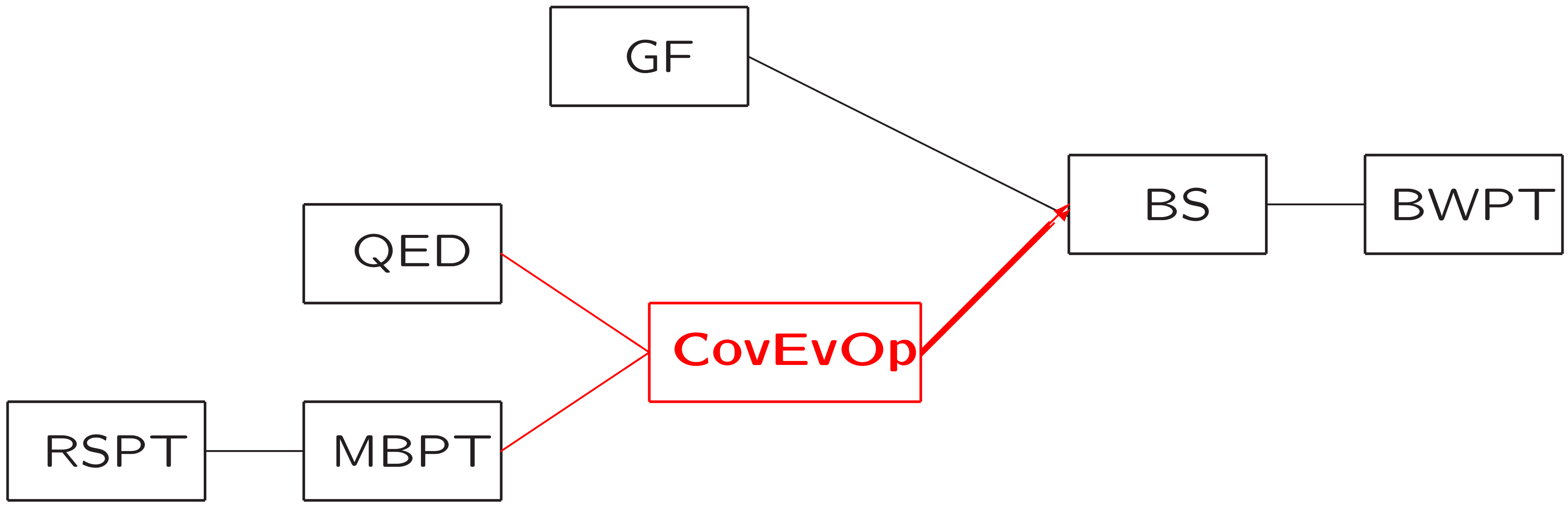
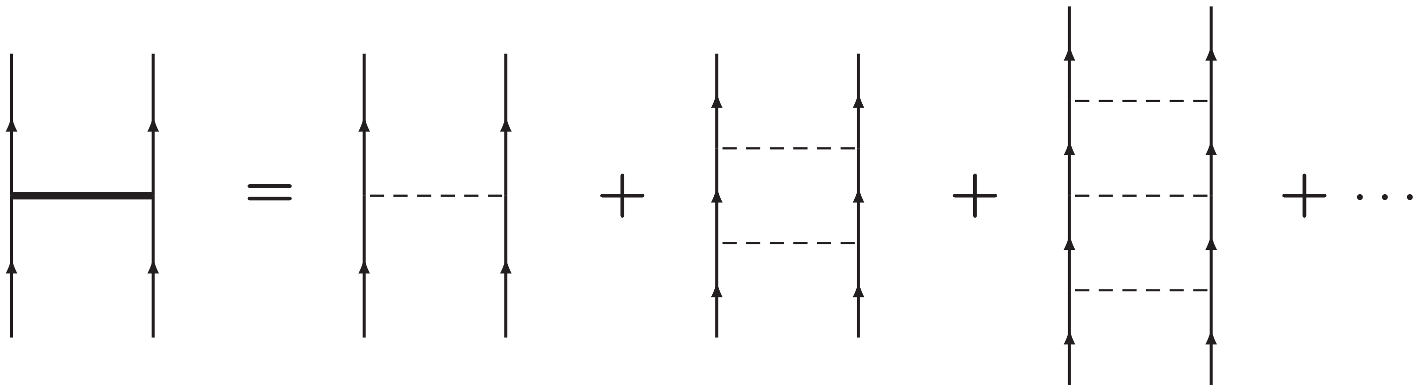
Can. J. Physics (2005)



Effective-potential method

Relativistic pair function



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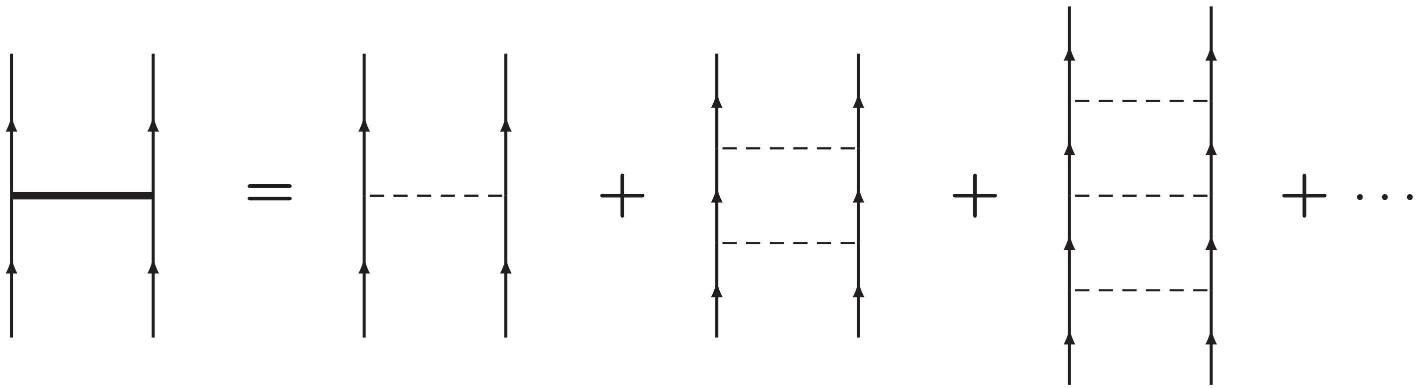
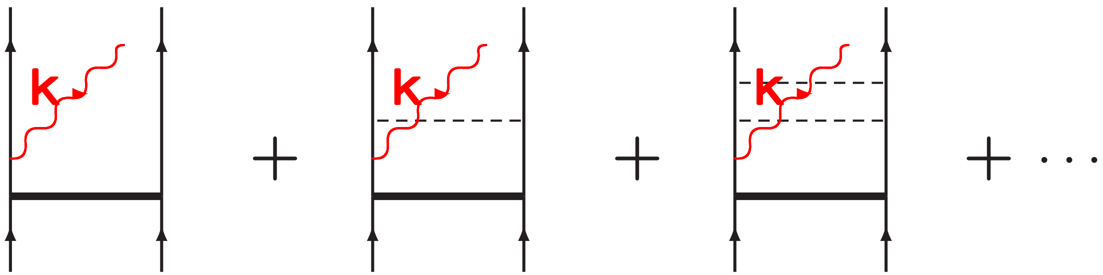
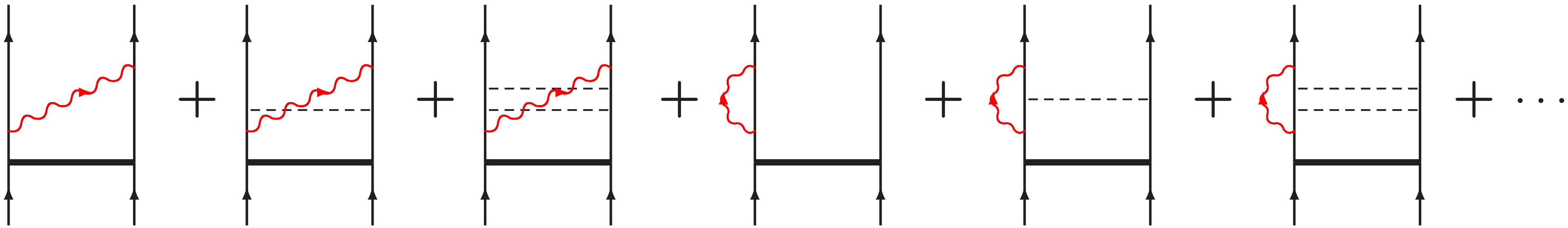


with an uncontracted photon



Absorb the photon and integrate over momentum



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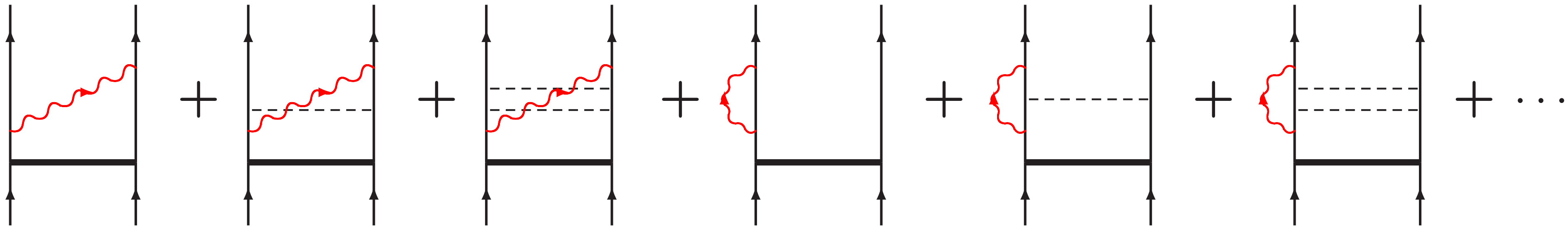
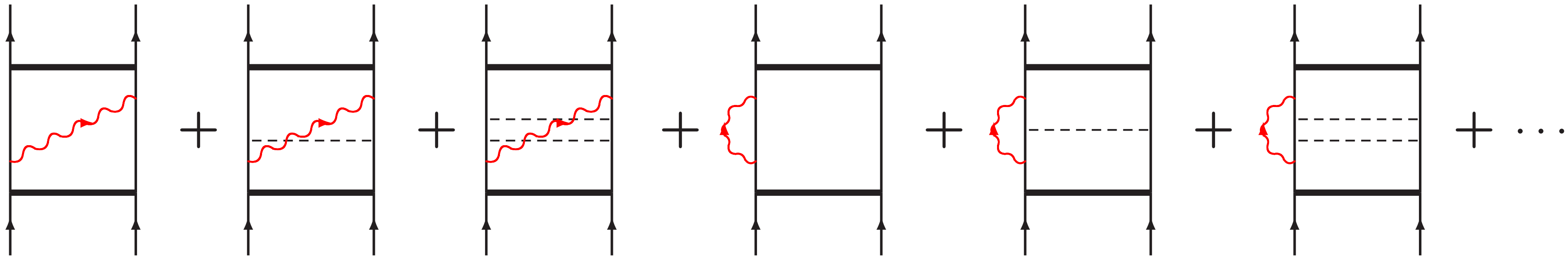


Pair functions iterated further



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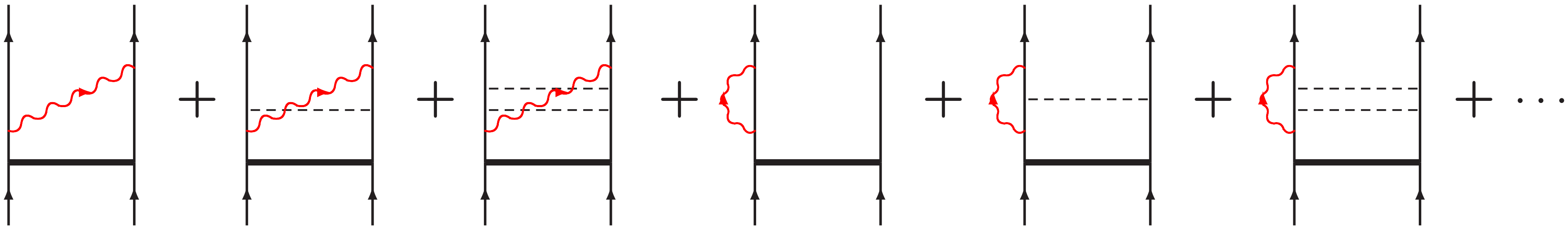

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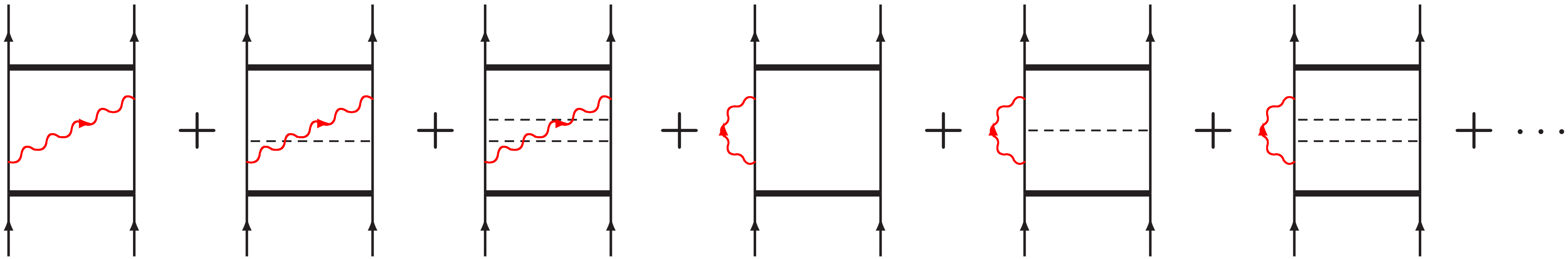
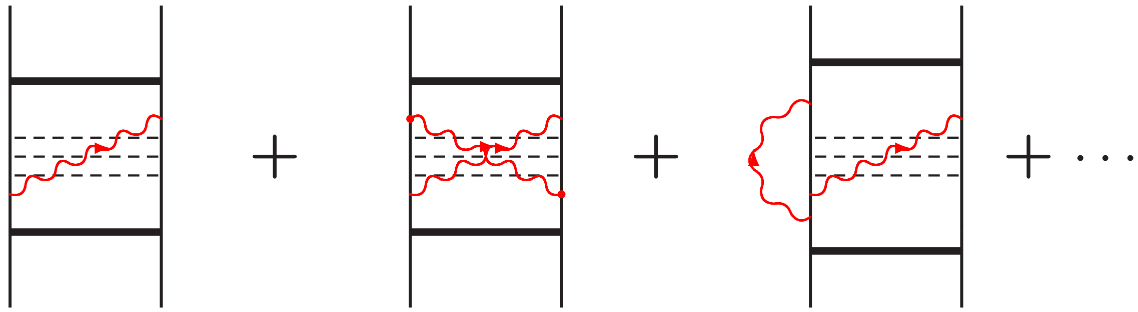
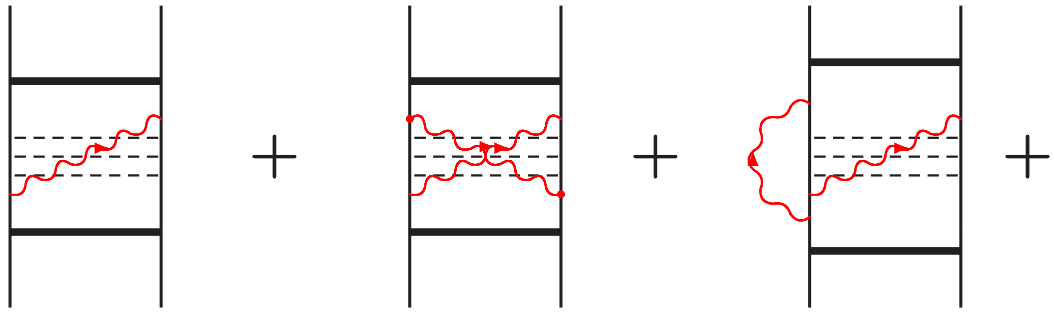


QED effects evaluated with correlated wave functions



non-separable (irreducible)

 $+ \cdots$

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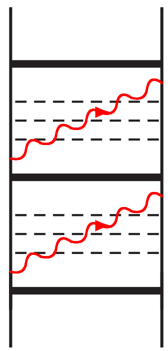
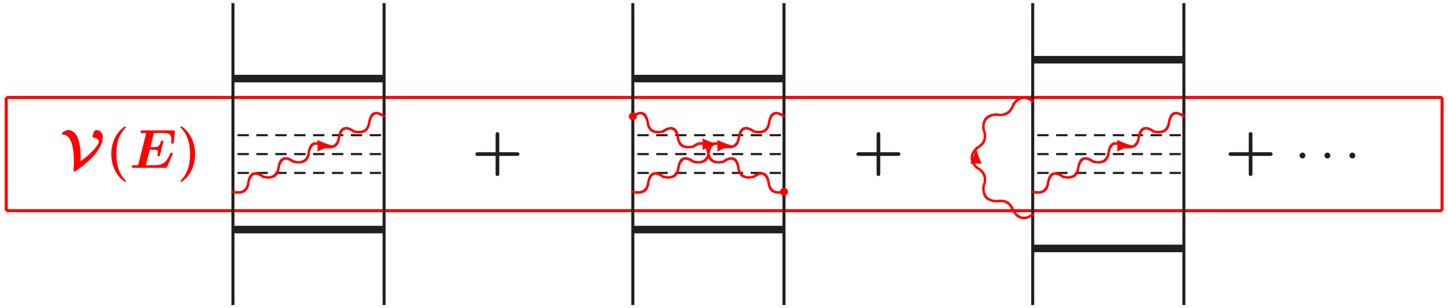
 $+ \cdots$

separable (reducible)

Effective potential



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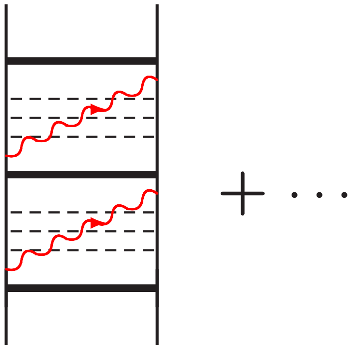
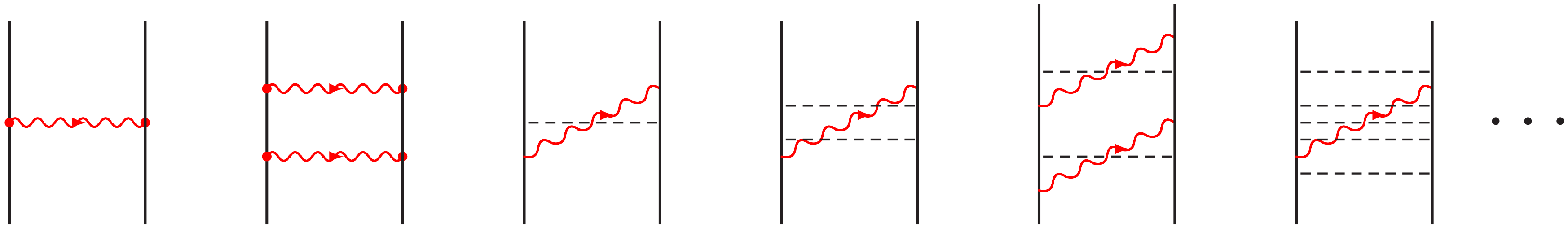


separable (reducible)

Effective potential

(with single covariant photon)



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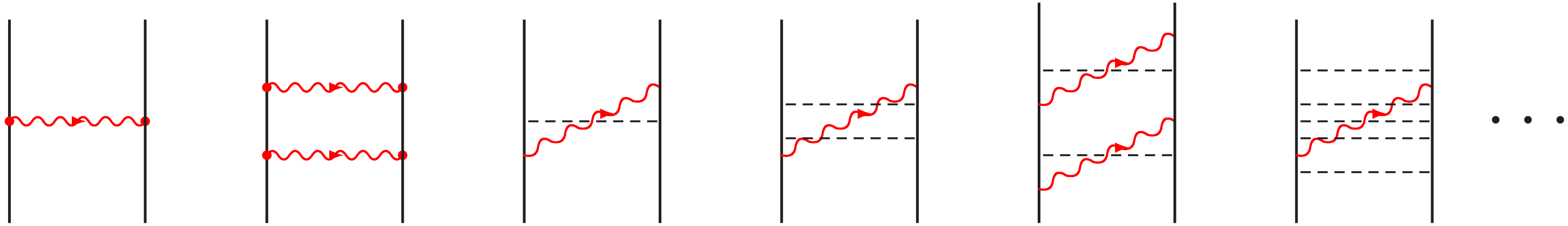
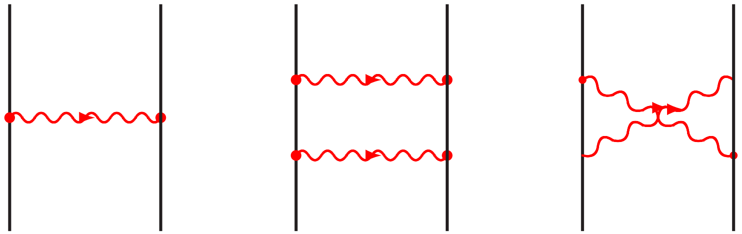


Comparison with S-matrix:

(with two covariant photons)



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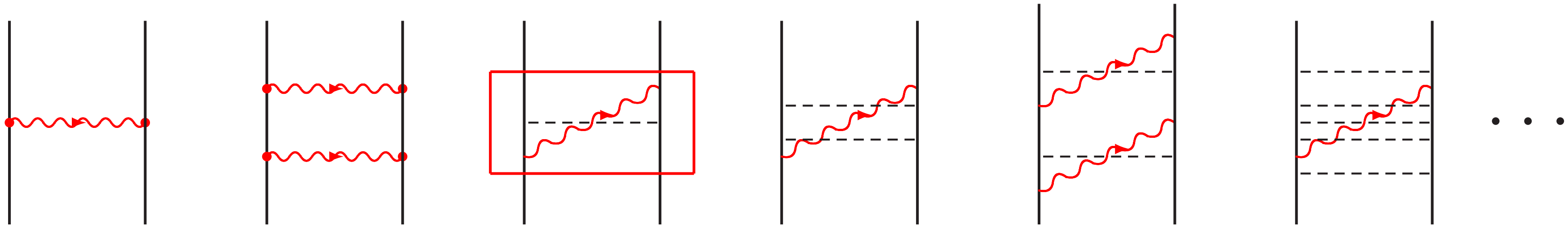

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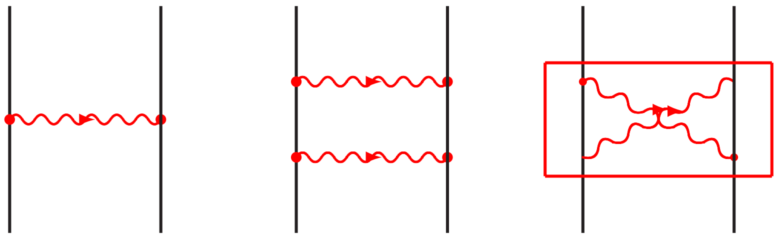

Two retarded photons (Breit-Breit) included in S-matrix approach

Test of new technique (in μH)

	Gr. state $1s^2$	
	S matrix	New technique
Coulomb-Gaunt NVP	-132.68	-132.61
Coulomb-Retardation NVP	20.17	20.14
Breit-Breit NVP		
Total NVP	-112.58	-112.47

	Exc. state $1s2s\ ^1S$	
	S matrix	New technique s
Coulomb-Gaunt NVP	-33.3	-33.2
Coulomb-Retardation NVP	1.2	1.2
Breit-Breit NVP		
Total NVP -112.47	-32.1	-32.0

Test of new technique (in μH)

	Gr. state 1s^2	
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Coulomb-Gaunt NVP	-132.68	-132.61
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Breit-Breit NVP	**-0.07**	
Total NVP	-112.58	-112.47

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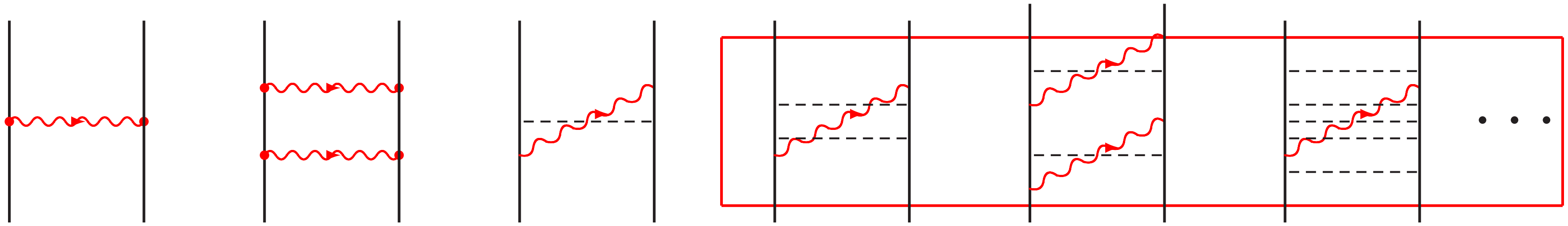

Comparison with S-matrix:
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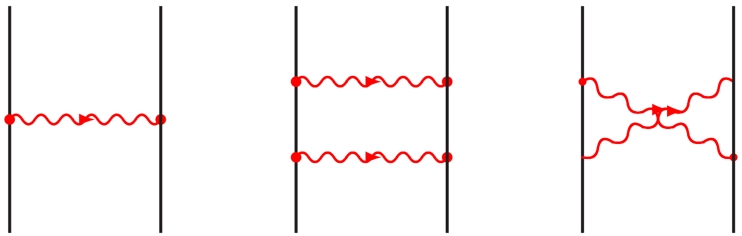
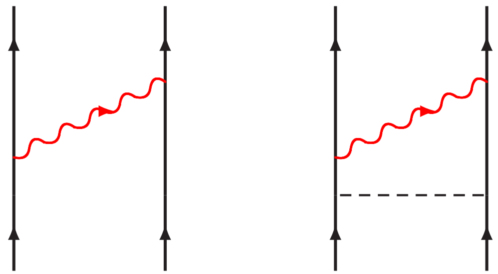


Dominating part of 3-, 4-, ... photon exchange
included in effective-potential approach

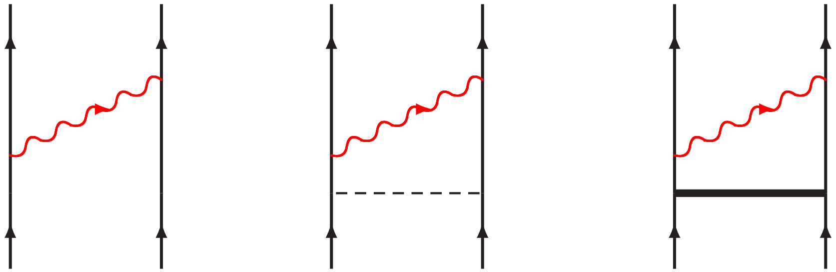
Effect of correlation on QED effect for helium atom



Interaction	Gr. state Sing. phot.	$1s^2$ two-phot.	multi-phot.
Gaunt	107	-65	
Scalar ret.	0	10	

Interaction	Exc. state Sing. phot.	1s2s ^1S two-phot.	multi-phot.
Gaunt	19.7	-16.6	
Scalar ret.	1.4	0.6	

Effect of correlation on QED effect for helium atom

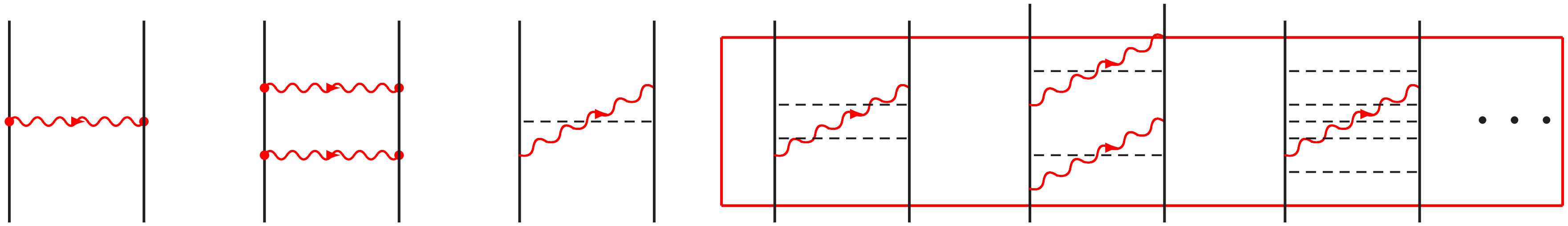


Interaction	Gr. state Sing. phot.	$1s^2$ two-phot.	multi-phot.
Gaunt	107	-65	**11**
Scalar ret.	0	10	**-2**

Interaction	Exc. state Sing. phot.	1s2s ^1S two-phot.	multi-phot.
Gaunt	19.7	-16.6	**4.7**
Scalar ret.	1.4	0.6	**-0.5**

Effective potential

(with single covariant photon)



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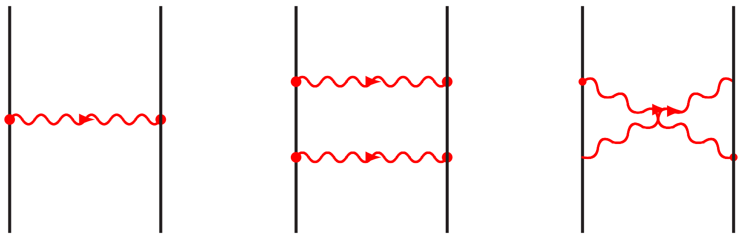

Effects beyond two-photon exchange orders of magnitude more important than Breit-Breit for light elements

The effective-potential approach leads faster to the Bethe-Salpeter equation:

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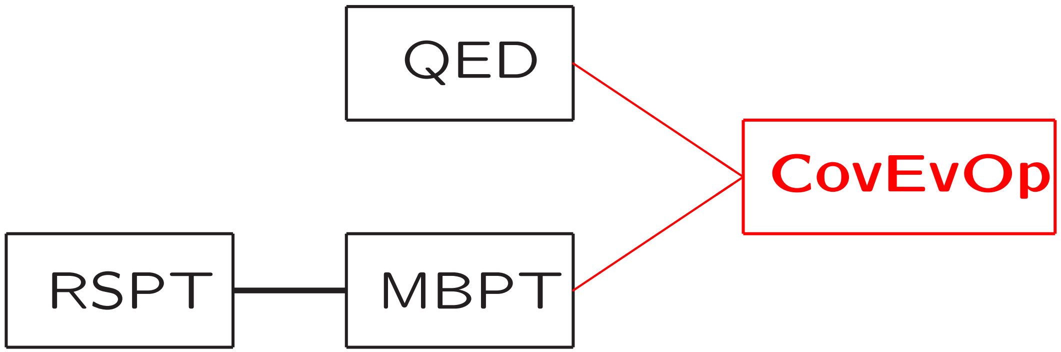
for treating **quasi-degeneracy**

Analogous to MBPT-Bloch equation:

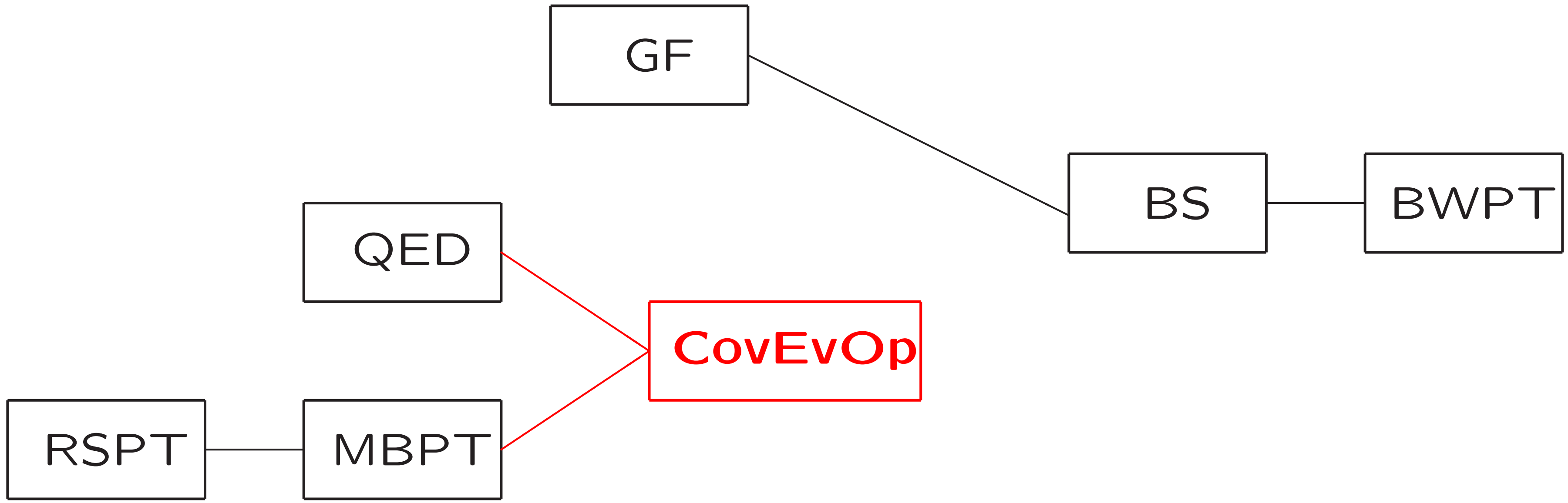
$$\left[\Omega, H_0\right]P = V\Omega P - \Omega\,PV\Omega\,P$$

MBPT-QED



MBPT-QED

Connection with Bethe-Salpeter Eq.



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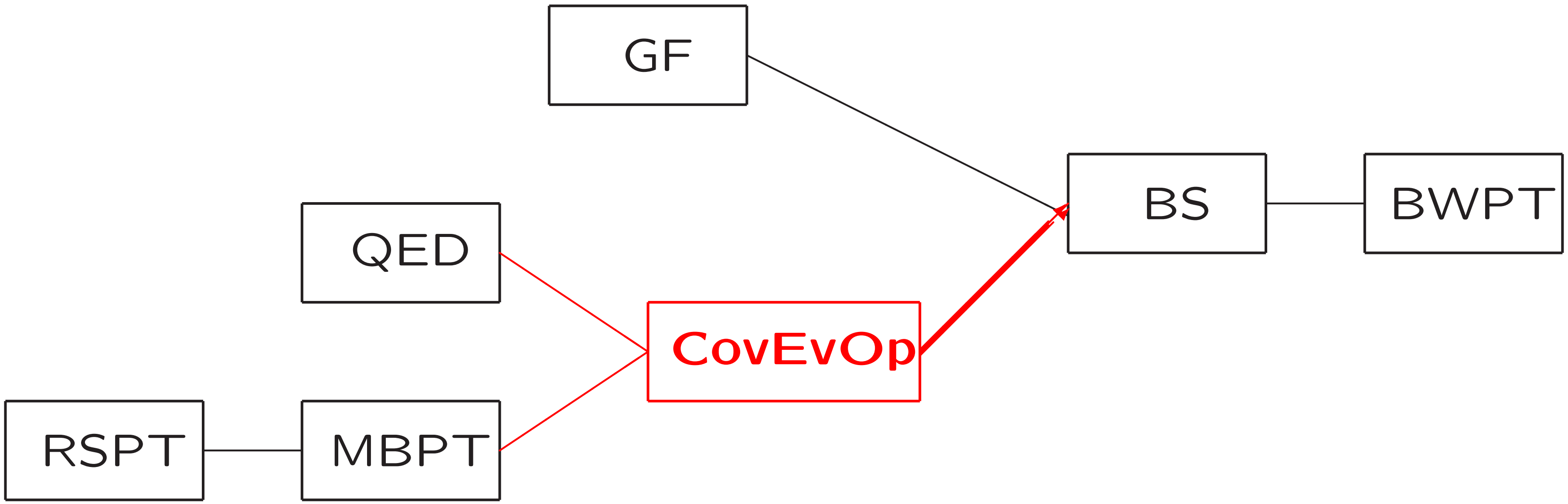
Can. J. Physics (2005)



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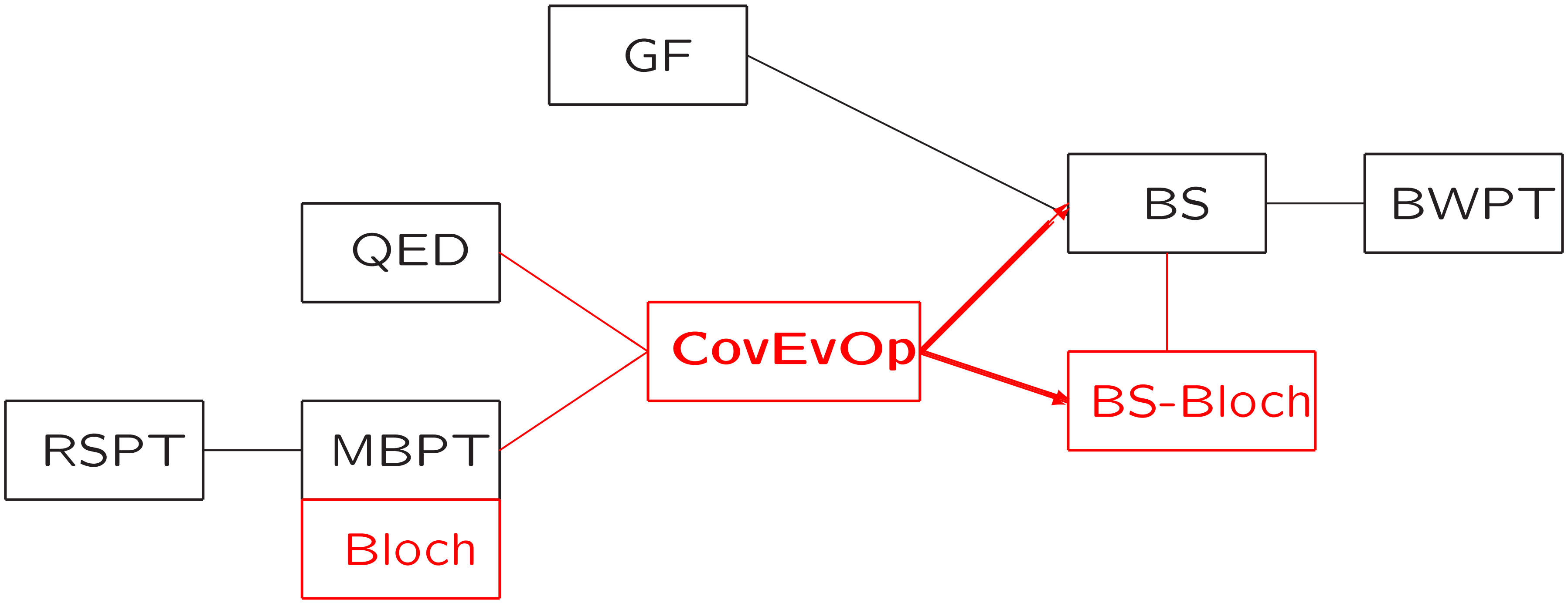

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3. Can contribute to extracting more accurate
fine-structure constant from the helium fine structure
by combining analytical and numerical techniques.

Fine-structure constant

(from Drake, Can. J. Phys. **80**, 1195 (2002))