Development of Many-Body Perturbation Theory

How to combine with Quantum ElectroDynamics?

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WHY?

Fundamental problem

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Very small effect in atomic/molecular physics

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First-order QED effects can be added to the ENERGY

OFTEN INSUFFICIENT

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Leads to a procedure where the QED effects are included perturbatively, mixed with the electron correlation - not added on at the final end

Outline

Review of standard methods

- Rayleigh-Schrödinger perturbation. Linked-diagram theorem. Bloch equation
- Relativistic MBPT. No-Virtual-Pair Approx.
- All-order methods. Coupled-cluster theory
- Methods for QED calculations

Outline

Beyond standard methods?

- Covariant Evolution Operator method
- Combination of MBPT and QED
- Numerical illustration: He-like systems
- Possible application to larger systems.
  Coupled-Cluster QED

MBPT Calculations

Standard non-relativistic MBPT

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

$$\Psi^\alpha = \boldsymbol{\Omega} \Psi_0^\alpha \quad (\alpha = 1 \cdots d) \quad \boldsymbol{\Omega} \text{ wave operator}$$

$$\Psi_0^\alpha = P\Psi^\alpha \quad \text{Intermediate normalization}$$

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Linked diagram theorem

Graphical representation:Unlinked diagrams cancel

(Brueckner 1955, Goldstone 1957, Brandow 1963, Mukherjee 1986)

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Bloch equation (Bloch 1958, IL 1974)

$$\boldsymbol{[\Omega, H_0]P = Q\big(V\Omega - \Omega W\big)_{\text{linked}}P}$$

$$\boldsymbol{-\Omega W} \qquad \text{Model-space contribution}$$

$$W = PV\boldsymbol{\Omega}P \quad \text{Effective interaction}$$

Model-space contribution

$$[\boldsymbol{\Omega}, H_0]P = Q\big(V\boldsymbol{\Omega} - \boldsymbol{\Omega}W\big)_{\rm linked}P$$

$$\text{Second order}: \ \ \boldsymbol{\Omega}^{(2)}P_{\mathcal{E}} = \Gamma_Q\big(V\boldsymbol{\Omega}^{(1)} - \boldsymbol{\Omega}^{(1)}P_{\mathcal{E}'}W^{(1)}\big)P_{\mathcal{E}}$$

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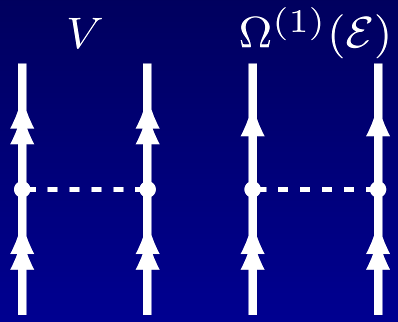
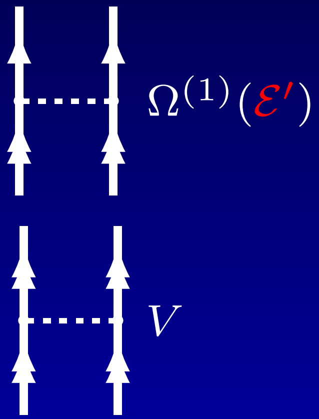


Unlinked



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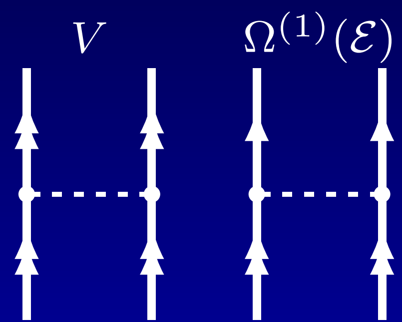

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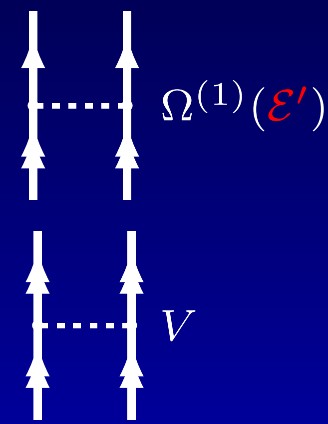
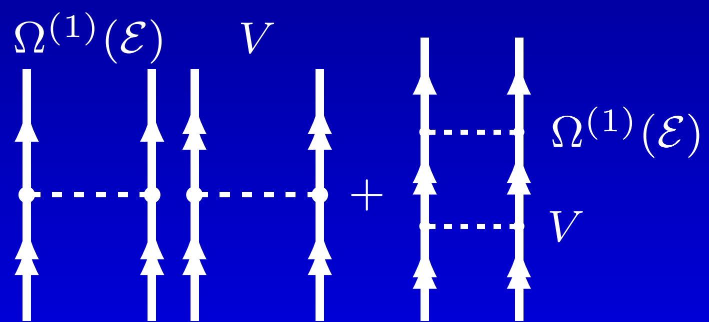
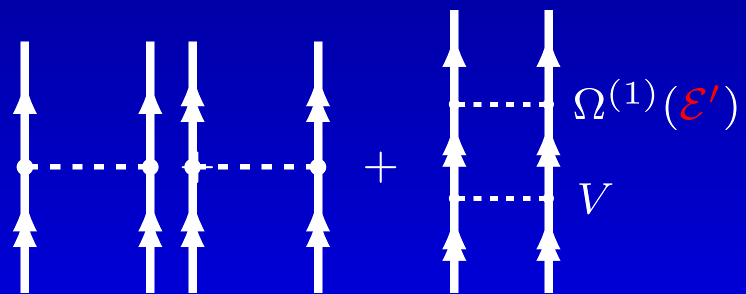




Unlinked Linked



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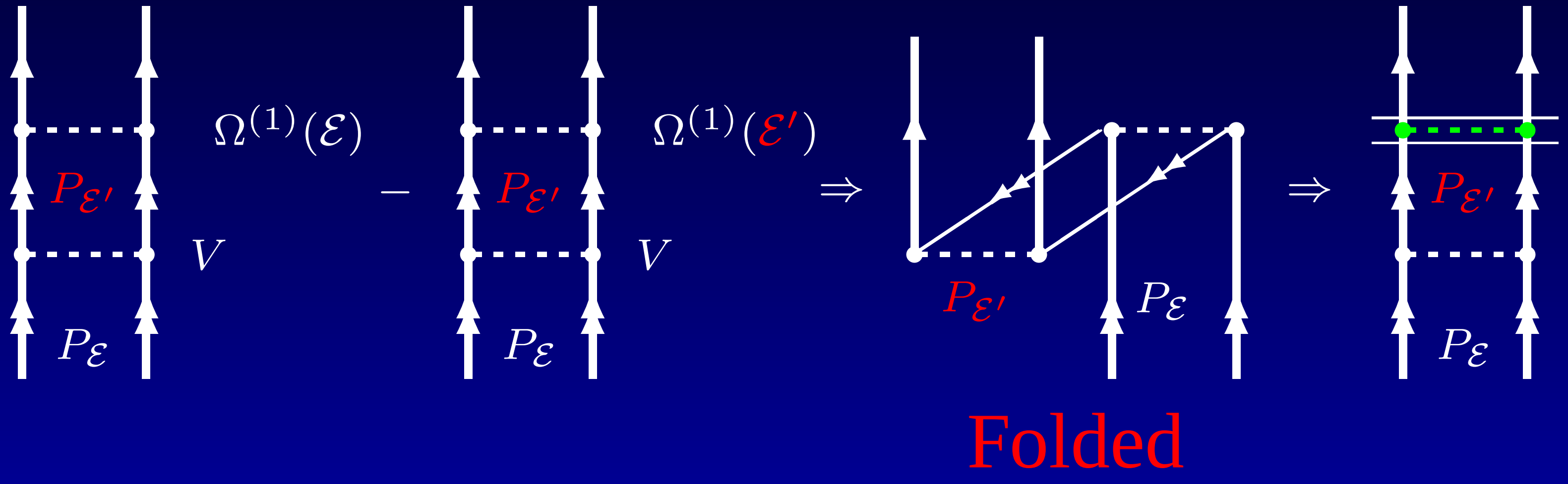
Remainder: Folded diagrams



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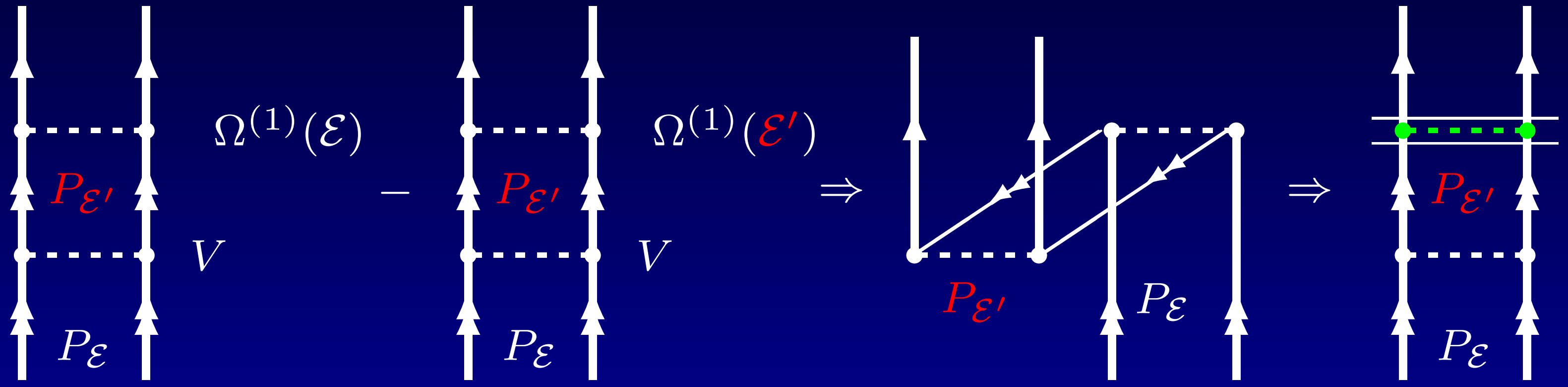

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$$\left(\Omega^{(1)}(\mathcal{E}) - \Omega^{(1)}(\mathcal{E}')\right) \frac{P_{\mathcal{E}'} V P_{\mathcal{E}}}{\mathcal{E} - \mathcal{E}'} = \frac{\delta\Omega^{(1)}}{\delta\mathcal{E}} \, P_{\mathcal{E}'} V P_{\mathcal{E}}$$

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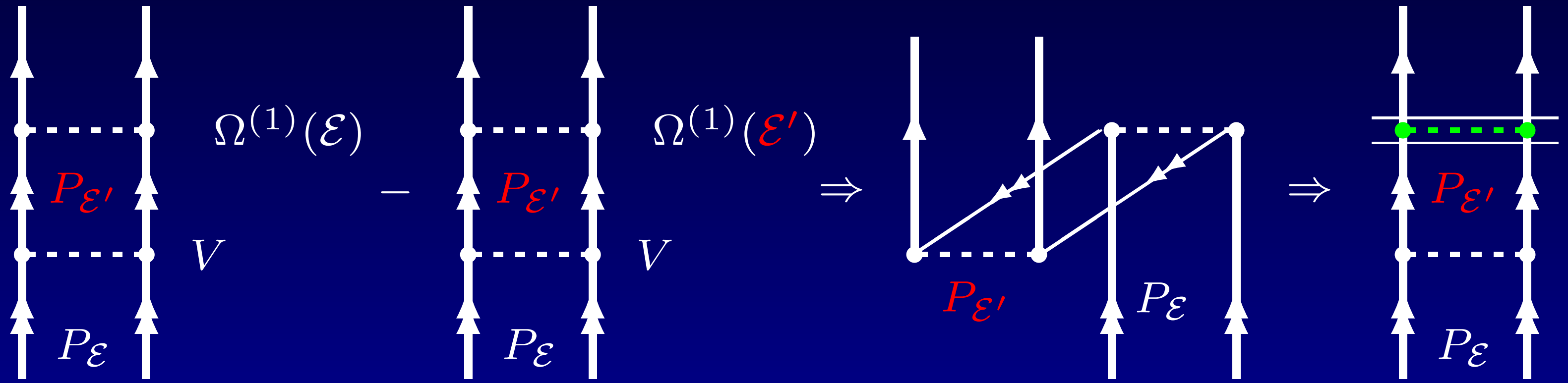

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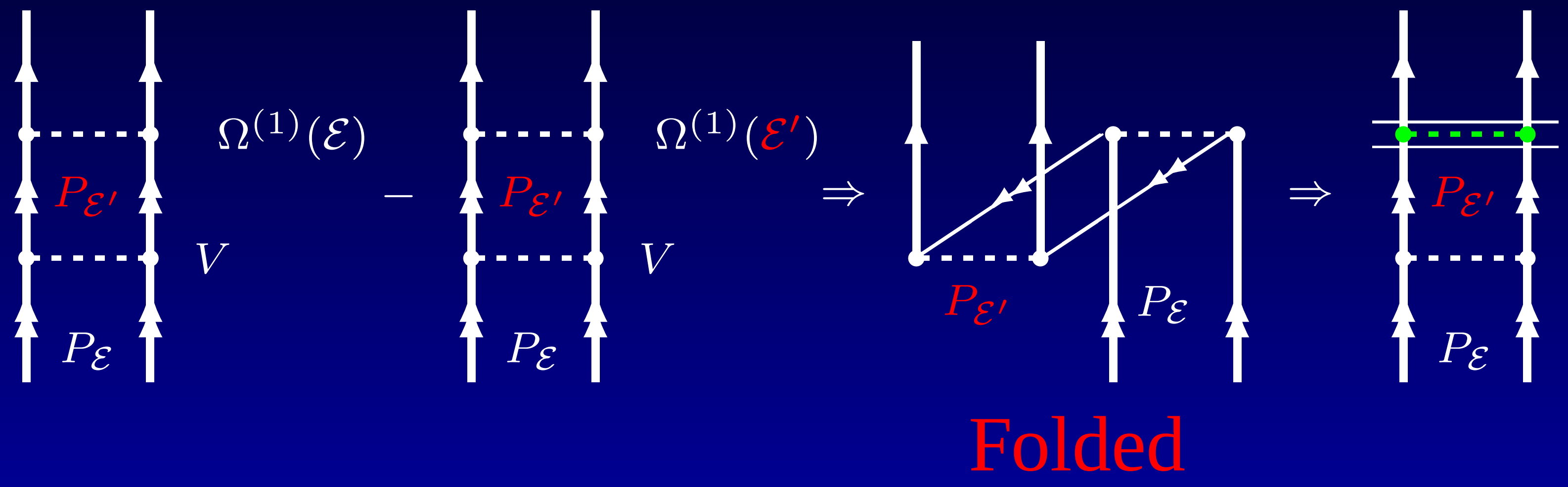

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$$\Omega^{(2)} = \Gamma_Q V \Omega^{(1)} + \frac{\delta\Omega^{(1)}}{\delta\mathcal{E}} W^{(1)} = \Gamma_Q V \Omega^{(1)} - \Gamma_Q \Omega^{(1)} W^{(1)}$$

$$\Omega = \Gamma_Q \big[V\Omega - \Omega W\big]_{\text{linked}}$$

Relativistic MBPT

(Breit 1931, Brown-Ravenhall 1951, Sucher 1980)

Dirac-Coulomb-Breit Approximation

$$H = \mathbf{\Lambda}_+ \Big[\sum_{i=1}^{N} h_{\boldsymbol{D}}(i) + \sum_{i<j}^{N} \frac{e^2}{4\pi r_{ij}} + H_B \Big] \mathbf{\Lambda}_+$$

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

Instantaneous Breit interaction

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Instantaneous Breit interaction

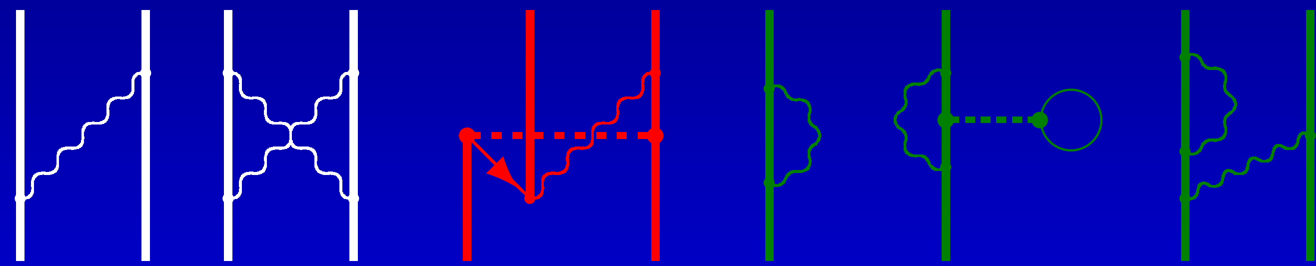
No-(virtual)-pair approximation (NVPA)

QED effects

Effects beyond NVPA - Energy dependent

Order α^3 and higher

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



Non-radiative effects   Radiative effects

All-order methods

$$\Omega = 1 + \Omega_1 + \Omega_2 + \cdots$$

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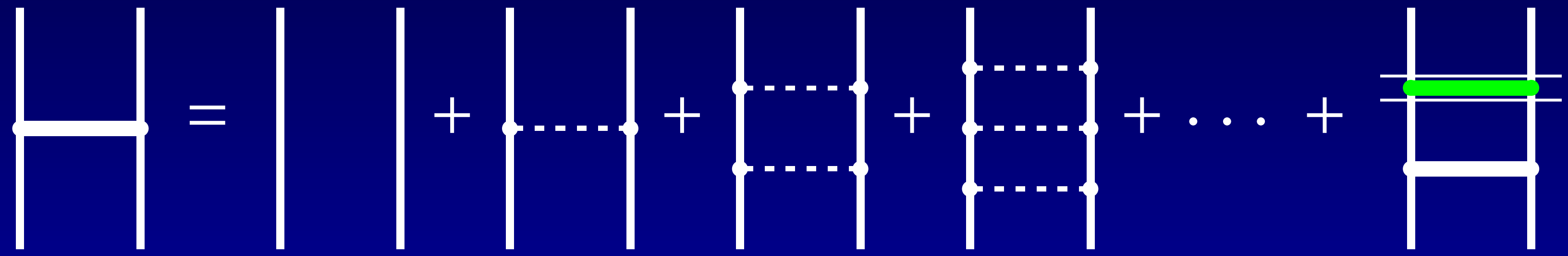
All-order pair function (Notre Dame, Gothenburg ...)

Ω_2 :



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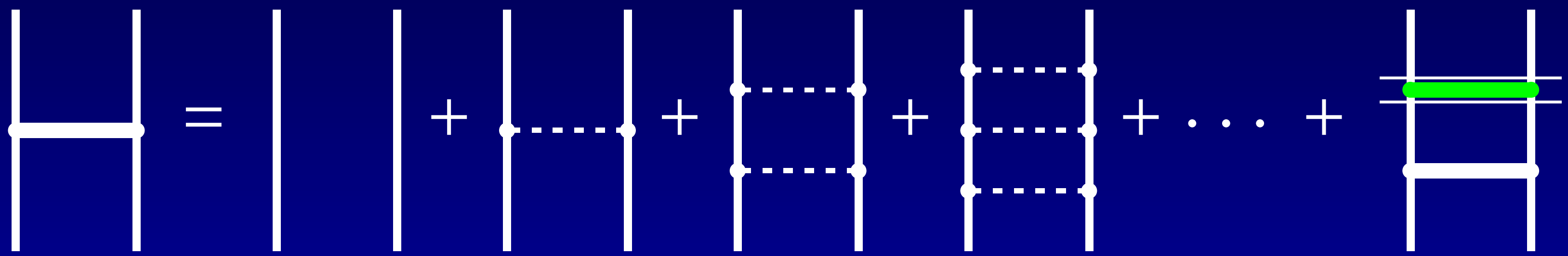

 Coulomb interaction

 Folded

Internal vertical lines: electron propagators w pos. and neg. electron states

Contains electron pair correlation to arbitrary order

Coupled-cluster approach

Exponential Ansatz (Coster 1958, Kümmel 1972, Čižek 1965)

Closed shells (single reference)

$$\Omega = \mathrm{e}^{T} = 1 + T + \frac{1}{2}T^2 + \frac{1}{3!}T^3 + \cdots$$

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Bloch equation

$$\big(E_0 - H_0\big)T = \big(V\Omega P - \Omega W\big)_{\mathrm{conn}}$$

Coupled-cluster approach

Normal-ordered exponential Ansatz

(IL1978, Mukherjee 1995, 97)

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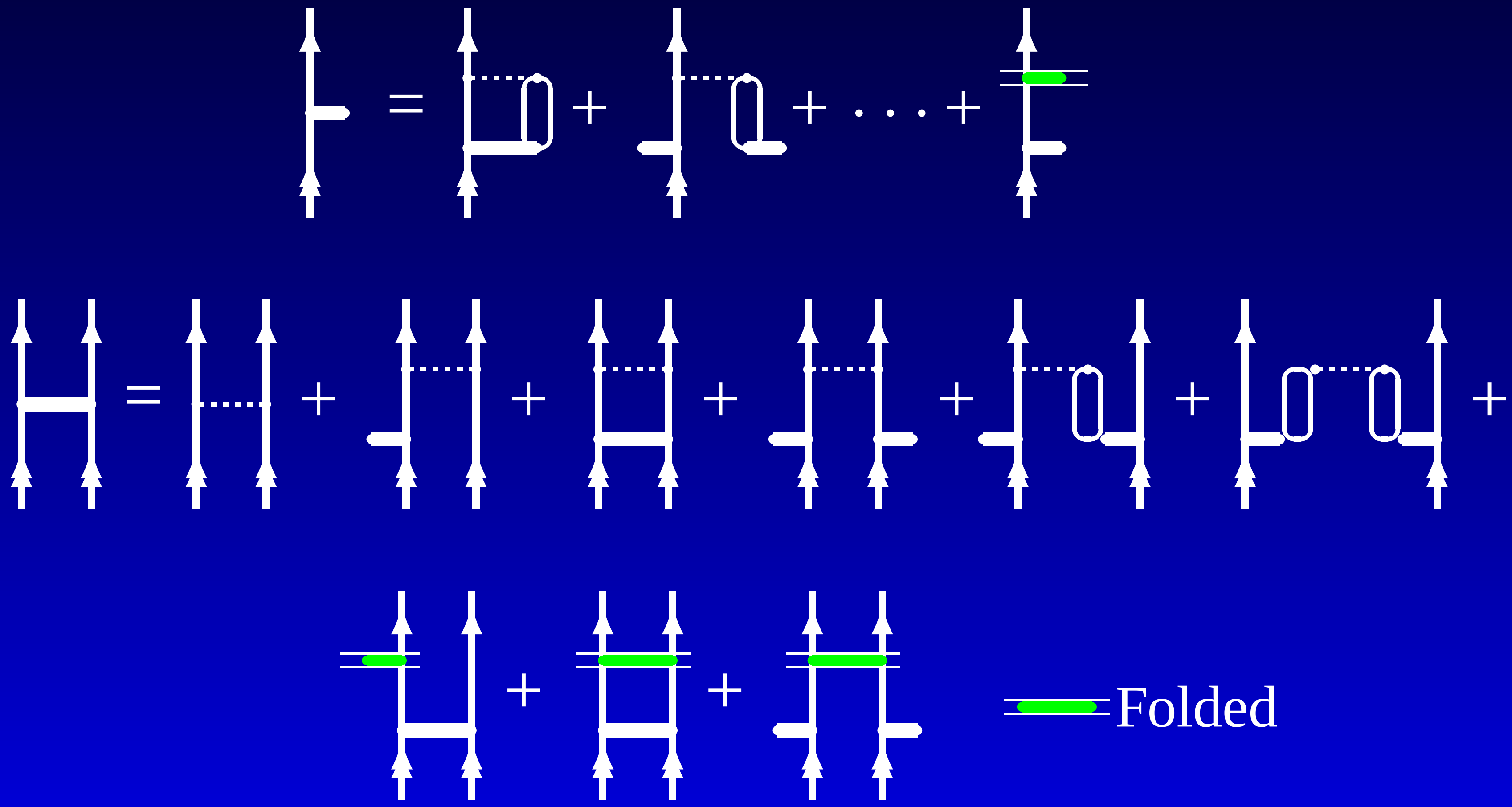

Numerical, closed shells

BH_3 molecule (Shavitt et al. 1972)

Ecxitations	Total	Connected	Disconnected
One-body	0.1	0.1	
Two-body	97.2	97.2	≤ 0.1
Three-body	0.8	0.8	≤ 0.01
Four-body	1.9	≤ 0.01	1.9

QED Calculations

Standard methods

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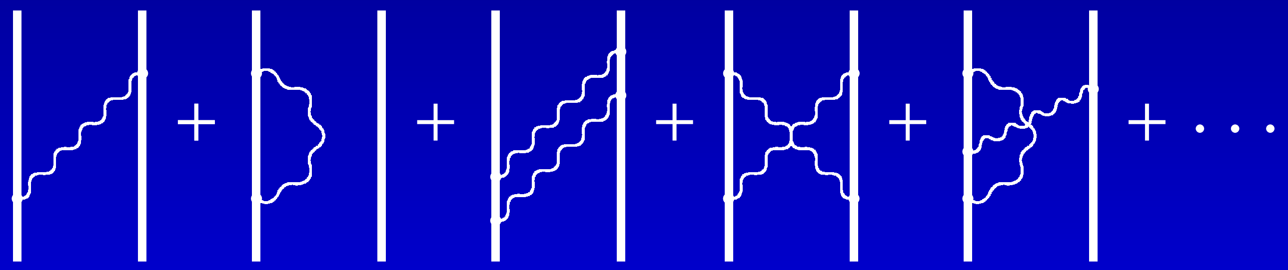

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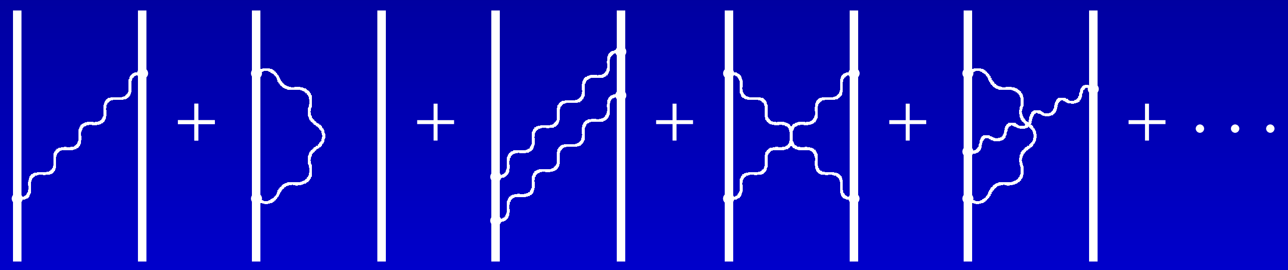

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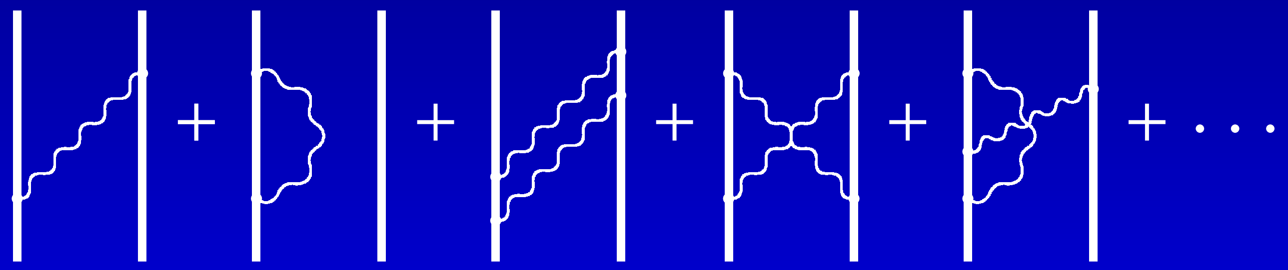

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CEO has similar structure as MBPT. Basis for unification

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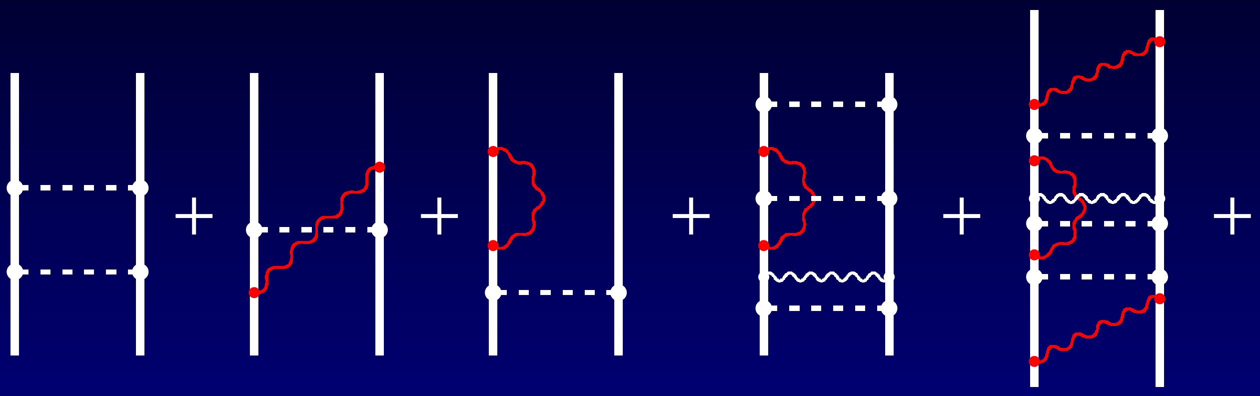
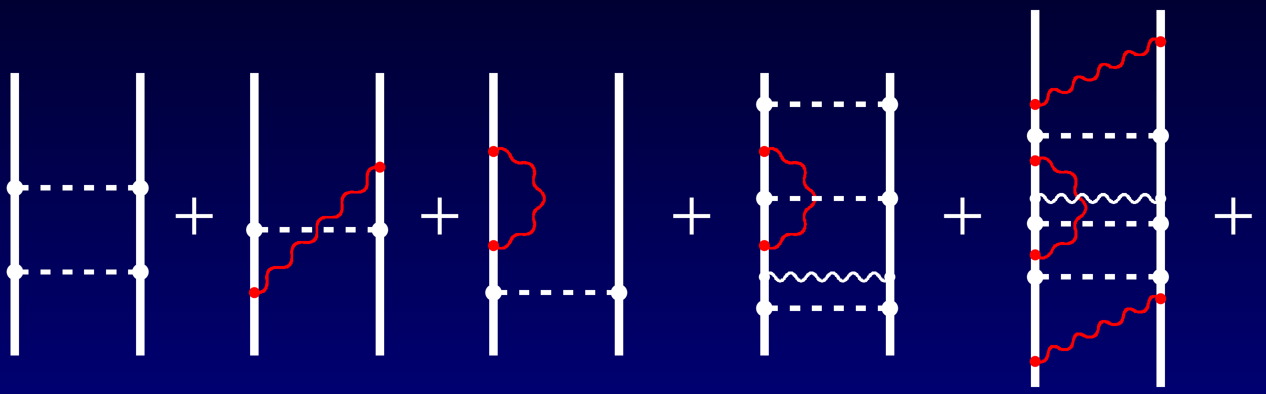
Employing time-dependent perturbation theory enables us to combine MBPT and QED

Makes it possible to treat QED and correlation perturbatively on the same footing

Time-dependent perturbation theory



Time-dependent perturbation theory



A procedure for time-dependent perturbation theory has been developed based upon the Covariant Evolution Operator (CEO) method

Time-dependent perturbation theory

Covariant Evolution Operator (CEO)

Time-dependent perturbation theory

Covariant Evolution Operator (CEO)

The single-particle Green-s function can be defined

(in Heisenberg representation, T Wick time ordering)

$$G(t,t_0)=\frac{\big\langle 0_{\rm H}\big|T[\hat{\psi}_{\rm H}(x)\hat{\psi}^{\dagger}_{\rm H}(x_0)]\big|0_{\rm H}\big\rangle}{\big\langle 0_{\rm H}\big|0_{\rm H}\big\rangle}$$

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The single-particle CEO analogously

$$U_{\rm Cov}(t,t_0)=\iint {\rm d}^3\boldsymbol{x}\,{\rm d}^3\boldsymbol{x}_0\,\hat{\psi}^\dagger(x)\langle 0_{\rm H}|T[\hat{\psi}_{\rm H}(x)\hat{\psi}^\dagger_{\rm H}(x_0)]|0_{\rm H}\rangle\hat{\psi}(x_0)$$

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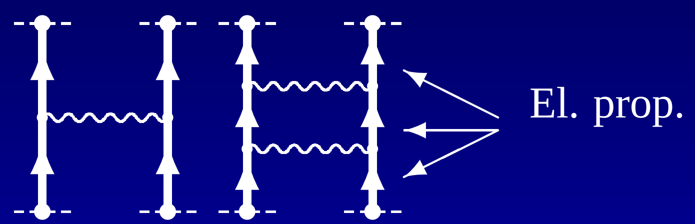

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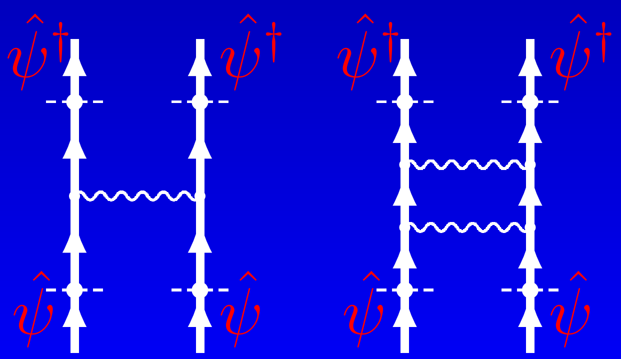

GF is a function

CEO is an operator

Time-dependent perturbation theory

Green's operator

Covariant evolution operator represents the time evolution of relativistic wave function

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

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Evolution operator singular due to intermediate model-space states

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Regular part known as Green's operator

$$U_{\mathrm{Cov}}(t,t_0)P = \mathcal{G}(t,t_0)\,PU_{\mathrm{Cov}}(0,t_0)P$$

Time-dependent perturbation theory

The Green's operator acts as the time-dependent relativistic wave operator

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

Time-dependent perturbation theory

Expansion of the Green's operator

$$U(t)P_{\mathcal{E}} = \mathcal{G}(t)\, P_{\mathcal{E}'} U(0) P_{\mathcal{E}}$$

$$\mathcal{G}^{(2)}(t) P_{\mathcal{E}} = Q\Big(\mathcal{G}^{(1)}(t)\, U^{(1)}(0) - \mathcal{G}^{(1)}(t) P_{\mathcal{E}'} U^{(1)}(0)\Big) P_{\mathcal{E}}$$

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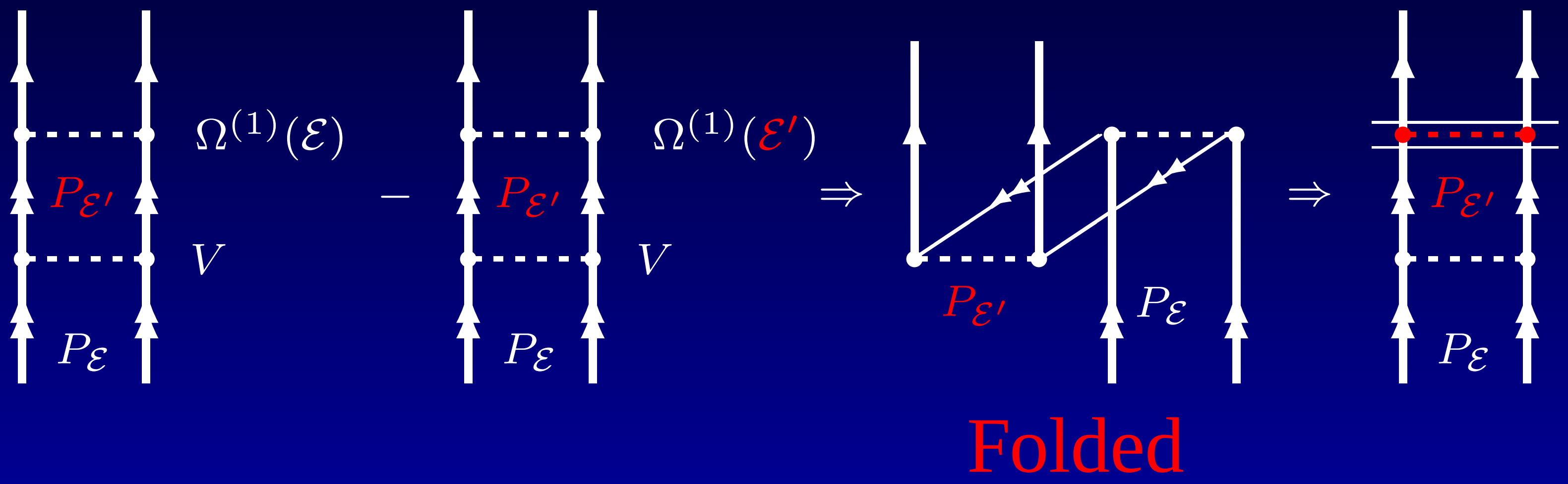
Compare std wave operator

$$\Omega P = \Gamma_Q \big(V\Omega - \Omega P W\big) P$$

$$\boldsymbol{\Omega}^{(2)} P_{\mathcal{E}} = \Gamma_Q \Big(V \boldsymbol{\Omega}^{(1)} - \boldsymbol{\Omega}^{(1)} P_{\mathcal{E}'} W^{(1)}\Big) P_{\mathcal{E}}$$

Time-dependent perturbation theory

Folded diagrams



$$\boldsymbol{\Omega}^{(2)} = \Gamma_Q V \boldsymbol{\Omega}^{(1)} + \frac{\delta\Omega^{(1)}}{\delta\mathcal{E}} W^{(1)} = \Gamma_Q V \boldsymbol{\Omega}^{(1)} - \Gamma_Q \boldsymbol{\Omega}^{(1)} W^{(1)}$$

Energy-independent perturbations

Time-dependent perturbation theory

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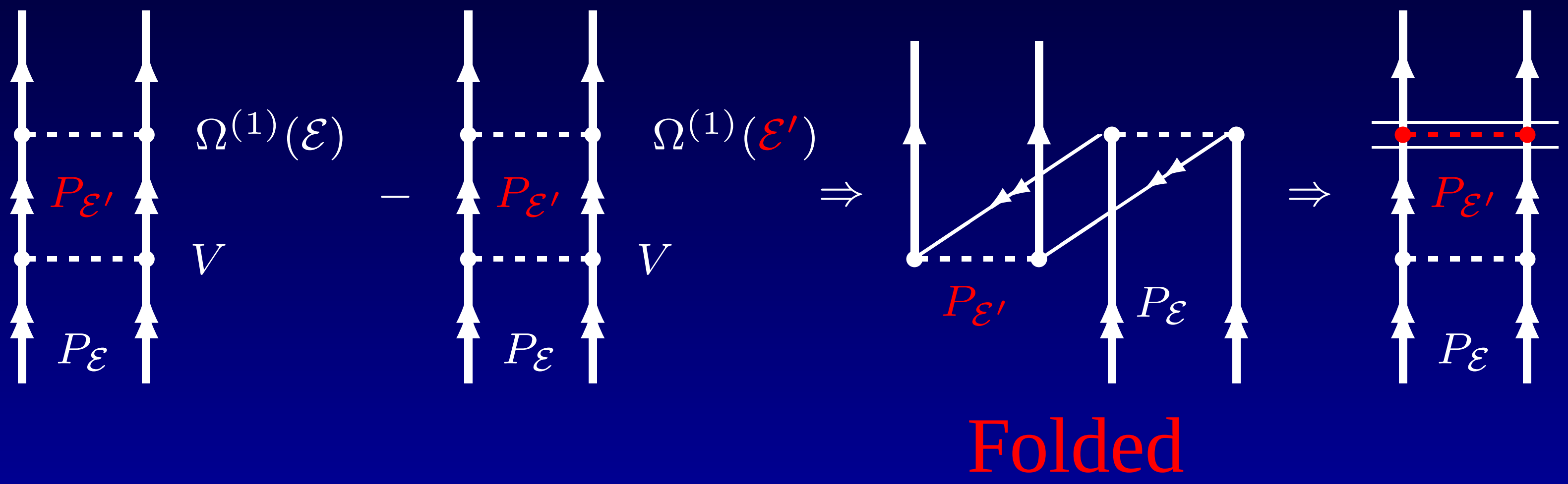

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Energy-dependent perturbations

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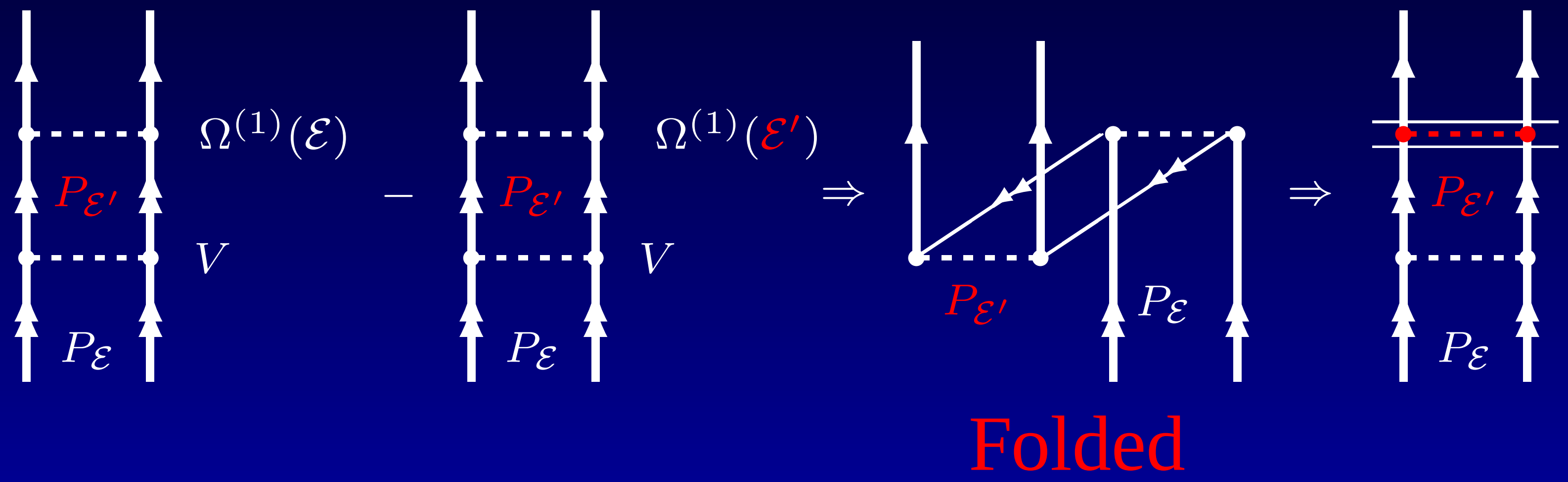

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Energy-dependent perturbations

Time-dependent perturbation theory

Bloch eqn for time-dependent perturbation theory

$$\left[\mathcal{G}, H_0\right] = V\mathcal{G} - \mathcal{G}W + \left[\frac{\delta^*\mathcal{G}}{\delta\mathcal{E}}, H_0\right] W$$

* derivation restricted to last interaction

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Procedures completely compatible

Time-dependent perturbation theory

How to evaluate the QED effects perturbatively?

Time-dependent perturbation theory

Gell-Mann-Low theorem

$$H_D|\Psi\rangle = \left(H_0 + V_C + v_T\right)|\Psi\rangle = E\,|\Psi\rangle$$

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$$V = V_C + v_T$$

Coulomb + Transverse

Time-dependent perturbation theory

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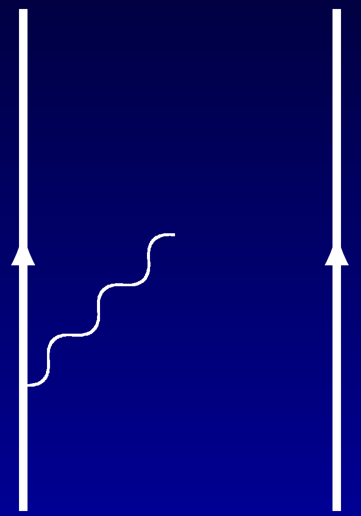
Coulomb + Transverse

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

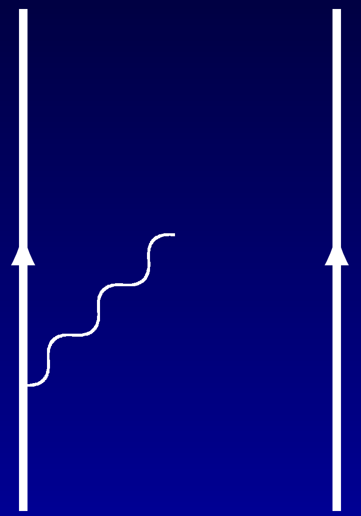
$$v_T = -\int \mathrm{d}^3x\,\hat{\psi}(x)^\dagger e c \alpha^\mu A_\mu(x)\hat{\psi}(x)$$

Time-dependent perturbation theory



Photonic Fock space

Time-dependent perturbation theory

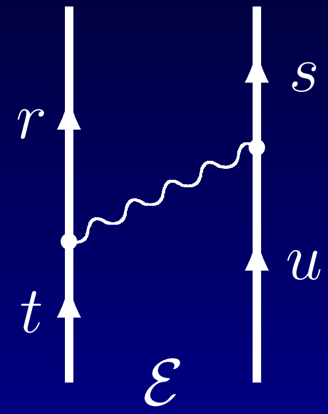


Photonic Fock space

Perturbation should be time independent!
for Gell-Mann-Low to be valid

Time-dependent perturbation theory

Single-photon exchange requires two perturbations



$$\langle rs|V_{\mathrm{sp}}(\mathcal{E})|tu\rangle = \left\langle rs\right| \int_0^\infty \mathrm{d}\kappa\, f(\kappa) \frac{1}{\mathcal{E} - \varepsilon_r - \varepsilon_u - \kappa} \left|tu\right\rangle$$

$$f(\kappa) = \sum_l V^l(\kappa \boldsymbol{r}_1) \cdot V^l(\kappa \boldsymbol{r}_2)$$

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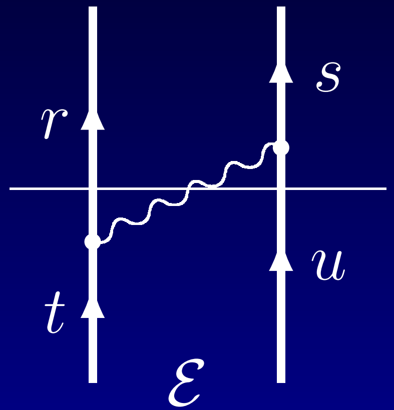

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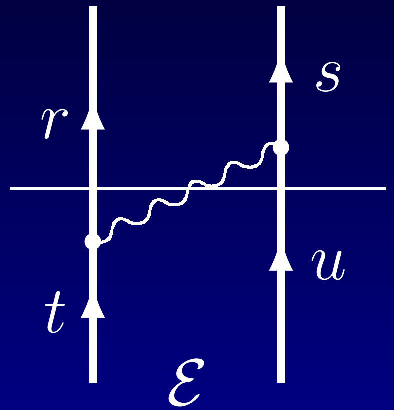

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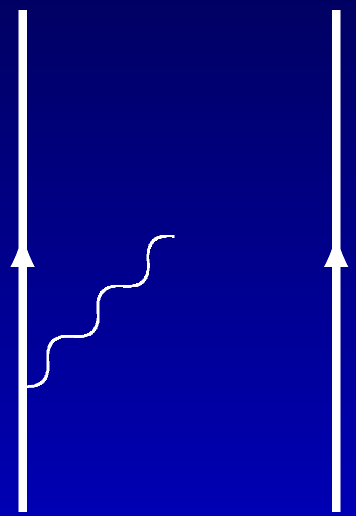
TWO energy-independent perturbations. The energy dependence is given by the energy denominator. GML valid

$$H_D\big|\Psi_l\big\rangle = \Big(H_0 + V_C + V^l\Big)\,\big|\Psi_l\big\rangle = E\,\big|\Psi_l\big\rangle$$

Time-dependent perturbation theory

Iteration of time-independent perturbations



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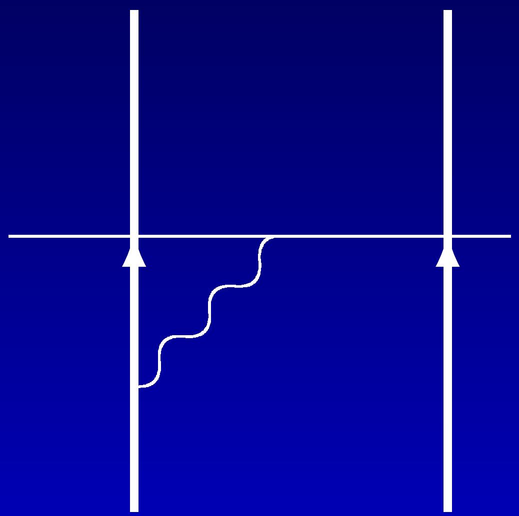

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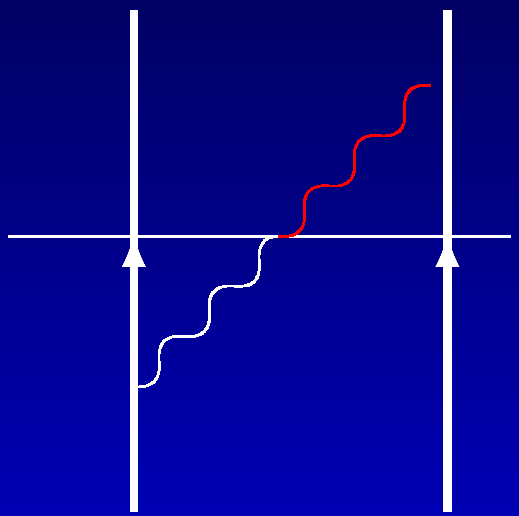

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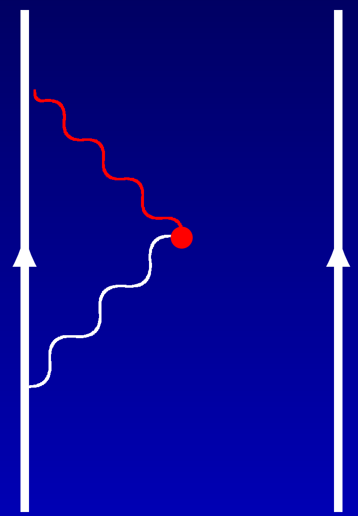

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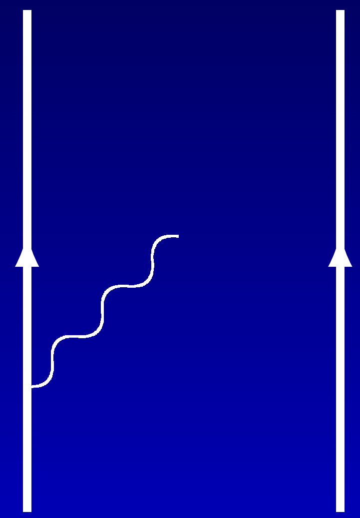

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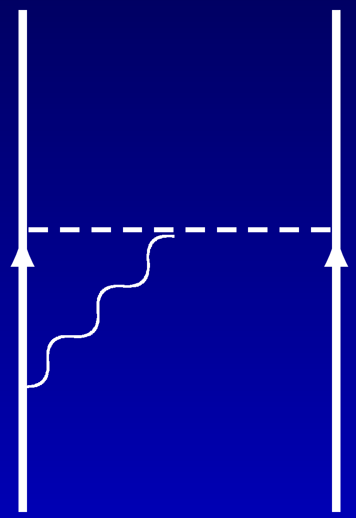

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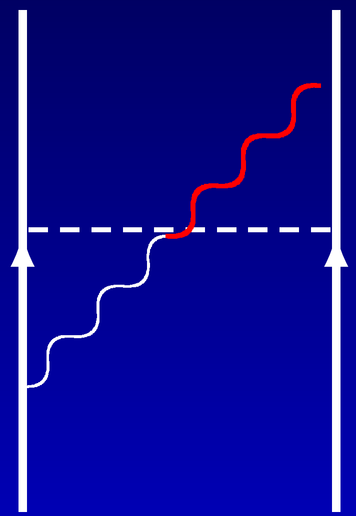

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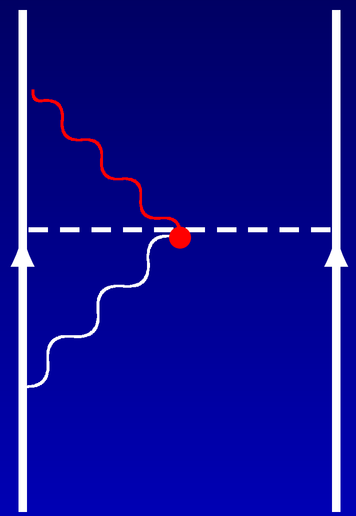
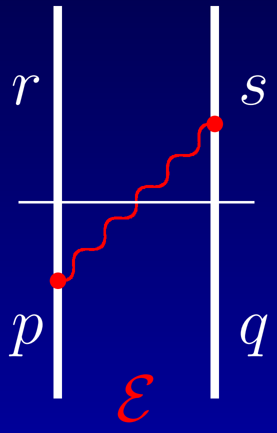


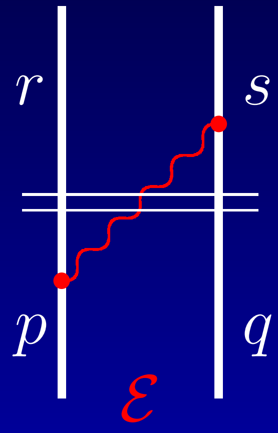
Time-dependent perturbation theory

Calculating derivative of retarded interaction



$$V = \frac{f(k)}{\mathcal{E} - \varepsilon_r - \varepsilon_q - k}$$

Derivative by second energy denominator

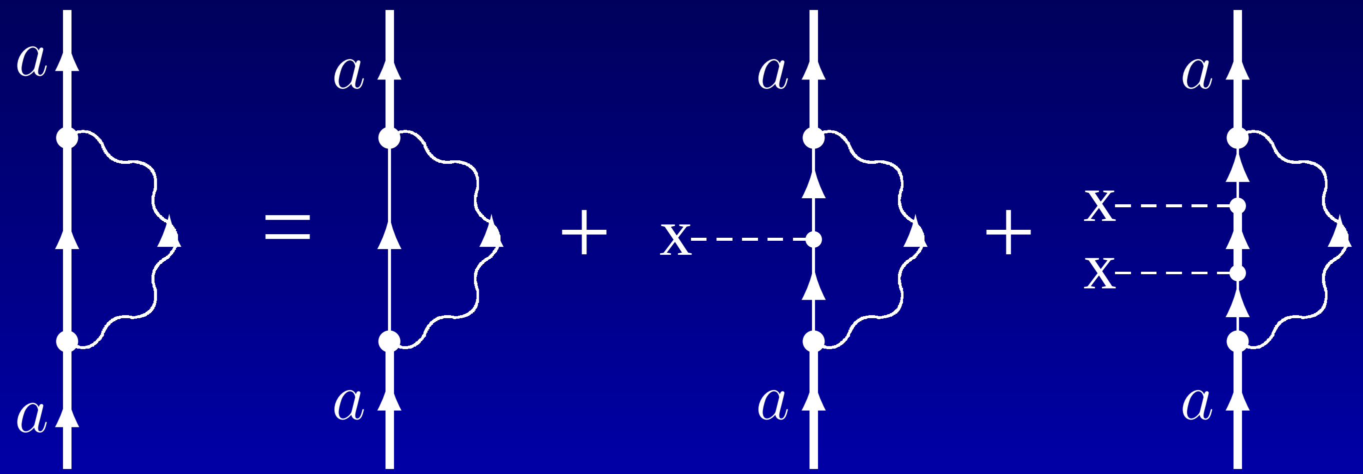


Self-energy regularization

Dimensional regularization in Coulomb gauge

most appropriate to use in MBPT/QED

Never used before.



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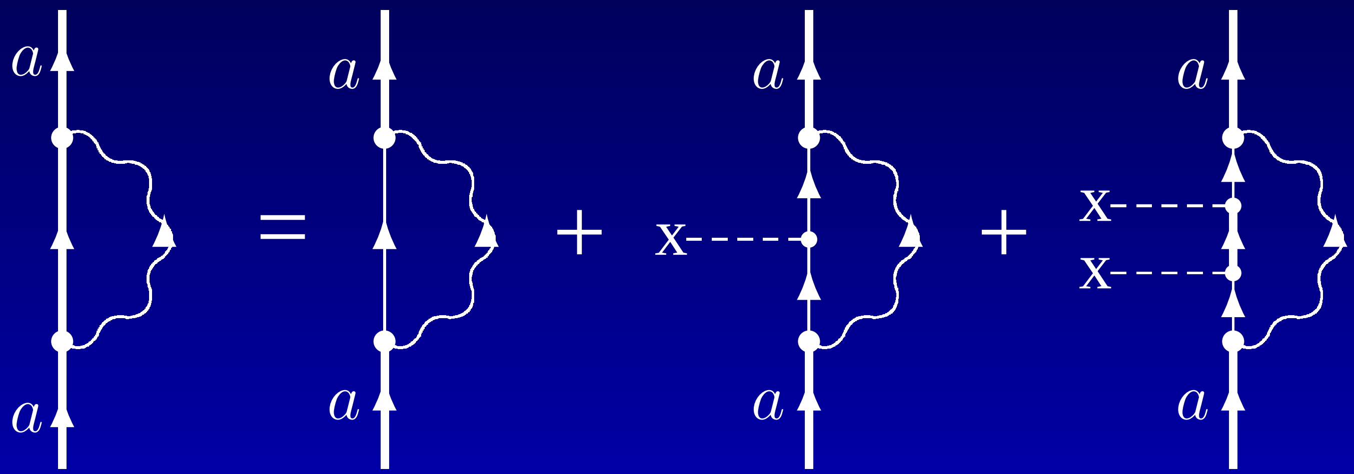

Zero- and one-pot. terms evaluated using Adkins formulas

Modified by J. Holmberg, PRA**84**, 062504 (2011)

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

Self-energy regularization

First dimensional regularization in Coulomb gauge

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)

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

Self-energy

Derivative of self-energy is singular
Singularity cancelled by vertex correction due to Ward identity

$$\frac{\delta \Sigma}{\delta \mathcal{E}} = \Lambda_0$$

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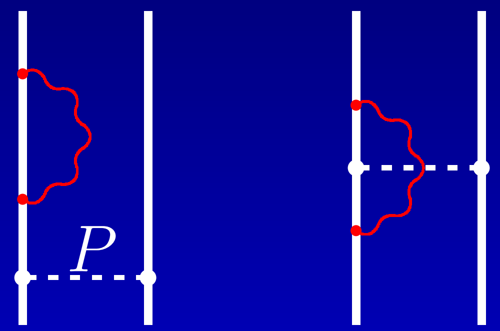
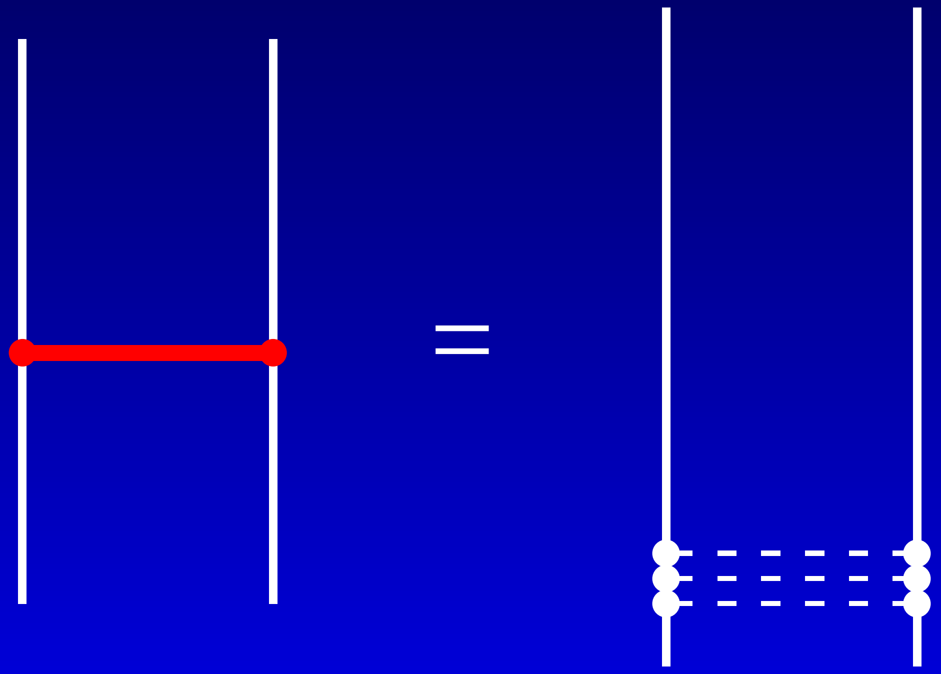


Both are charge divergent and have to be renormalized

Time-dependent perturbation theory

Iteration of time-dependent perturbations

QED Pair function



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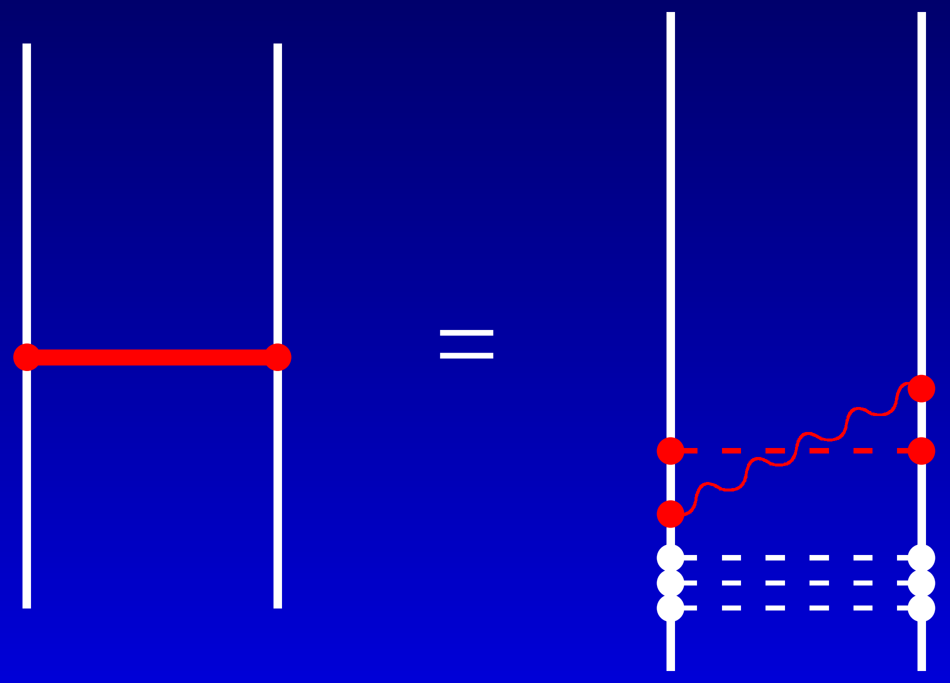

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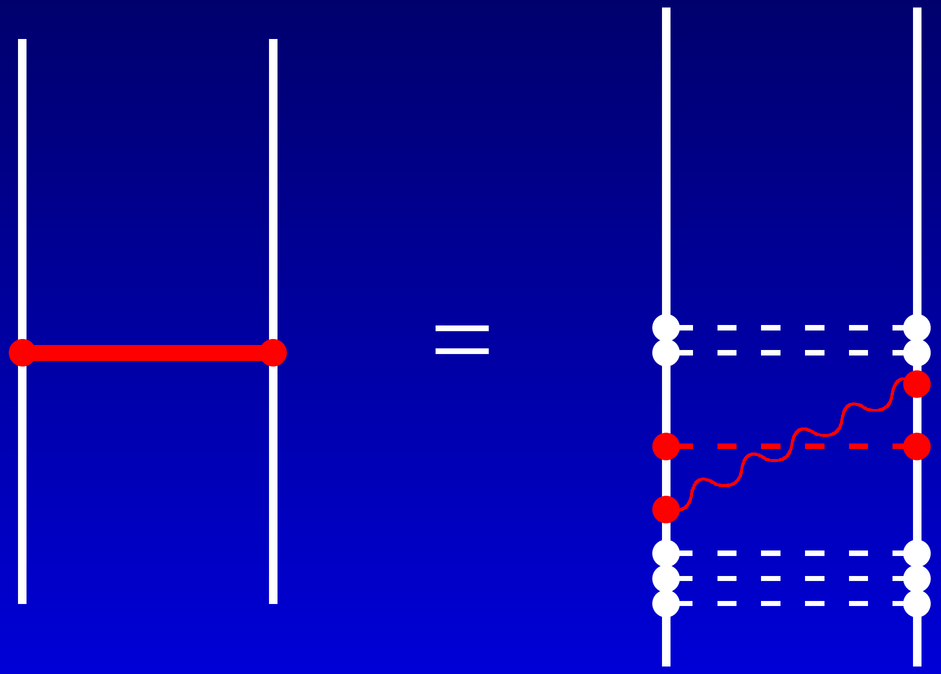

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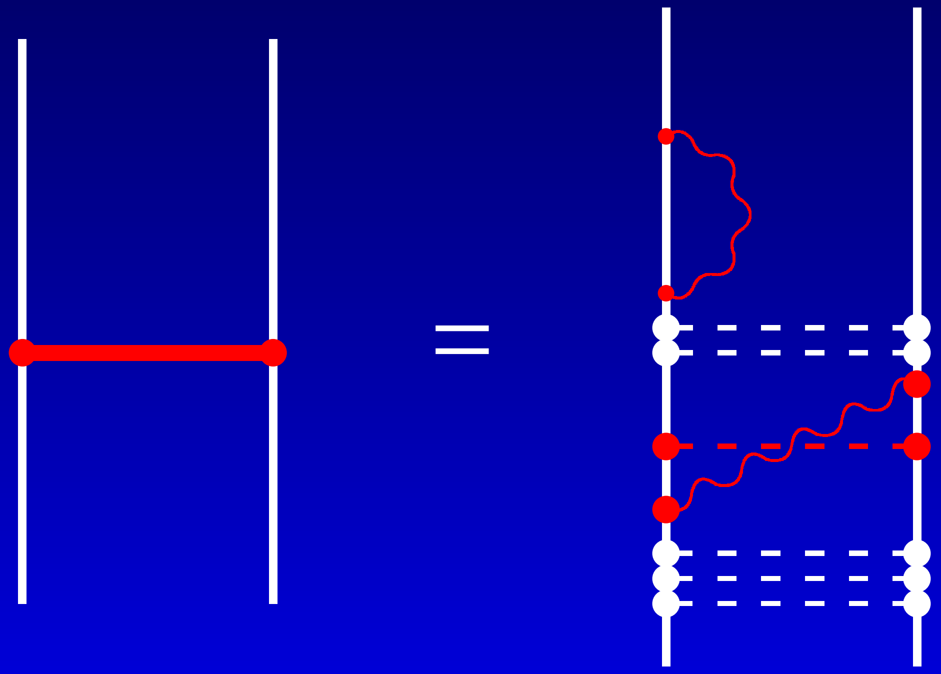

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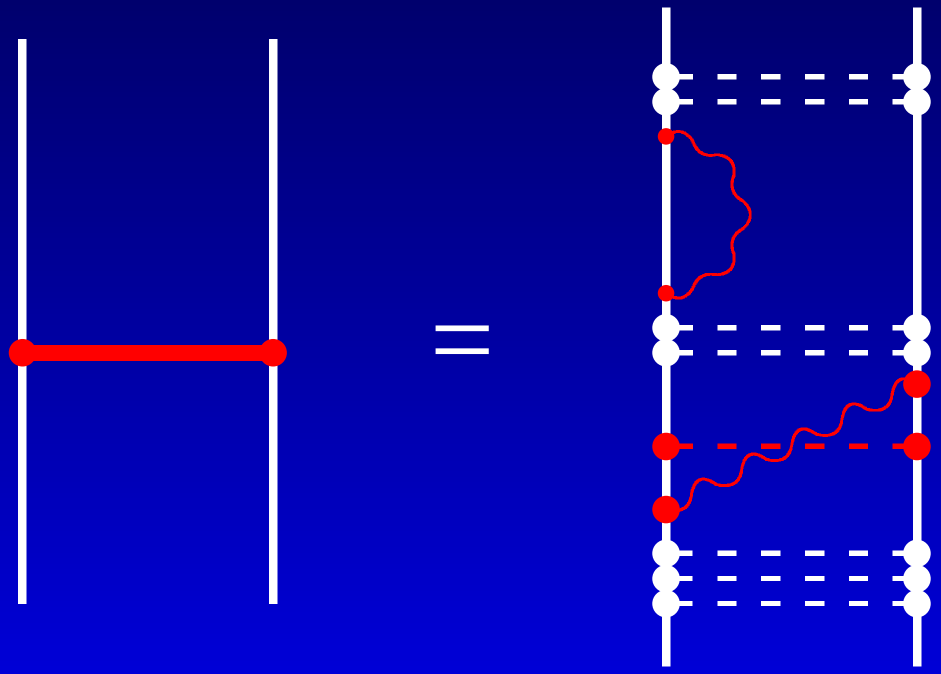

Numerical illustration

QED effects in He-like ions, grd state (eV)

Z	Two-photon	Combined QED-correlation BEYOND two-photon				
	Retarded	Inst. Breit	Retard. part	Virt.Pairs	Self-energy	Vertex corr.
10	0.0033	0.0072	-0.0011	0.0002		
14	0.0080	0.0101	-0.0019	0.0004	0.0020	
18	0.0150	0.0154	-0.0027	0.0006	0.0030	
24	0.0305	0.0192	-0.0042	0.0009	0.0050	
30	0.052	0.0244	-0.0057	0.0013	0.0090	
42	0.112	0.0286	-0.0087	0.0019		
50		0.0320	-0.011	0.0024	0.0170	
66		0.0400	-0.015	0.0030		

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Might have the potential, since the standard and QED procedures are completely compatible

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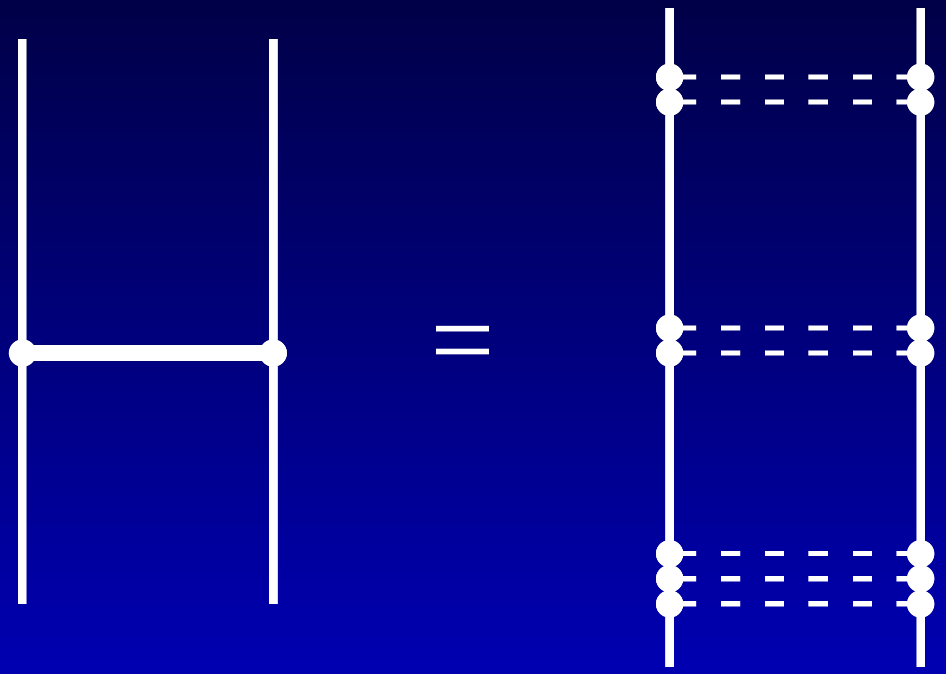
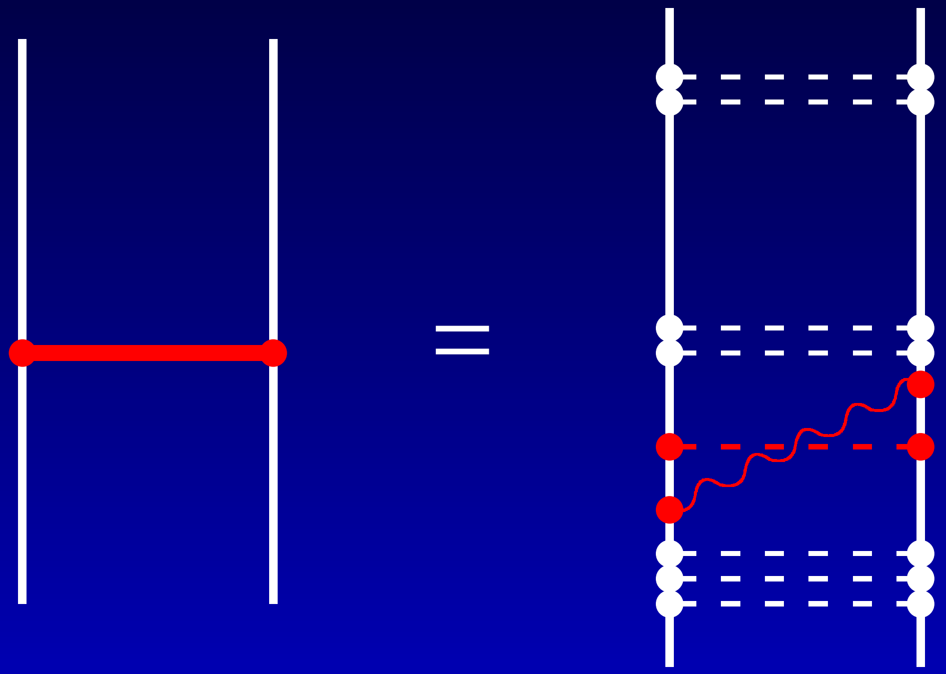
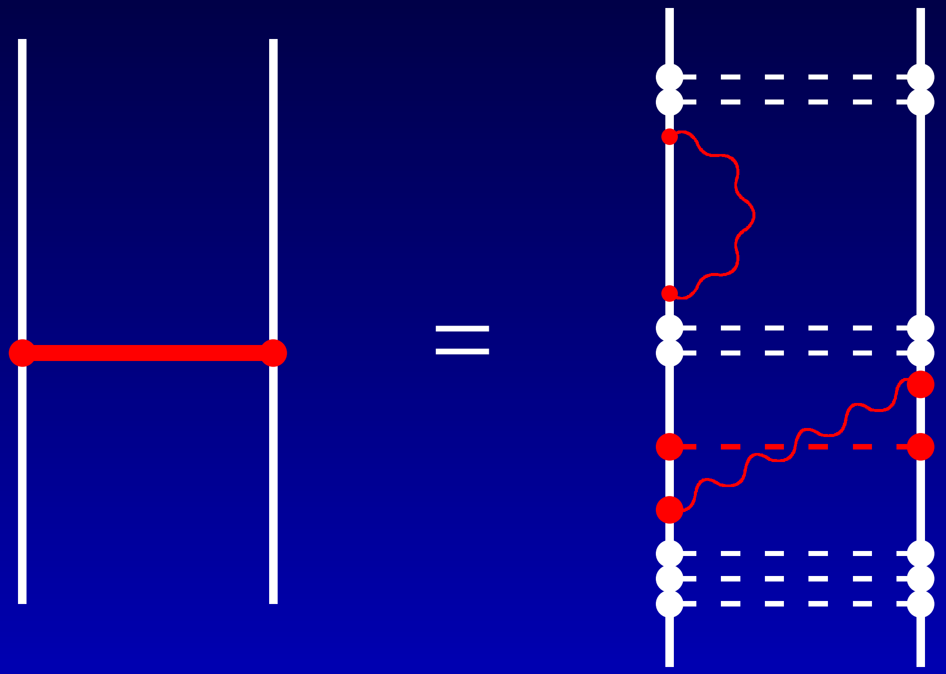
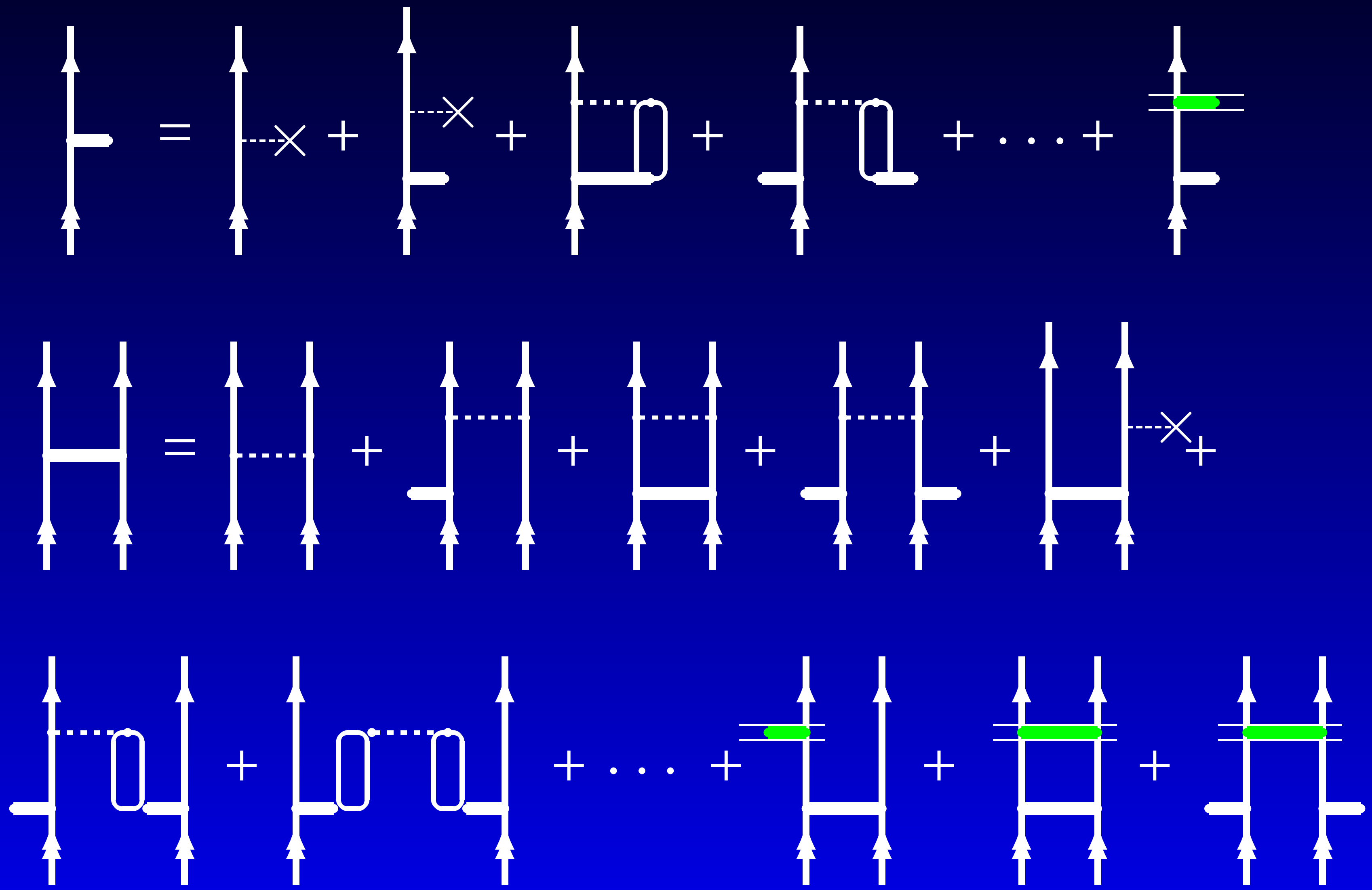






Coupled-cluster CCSD



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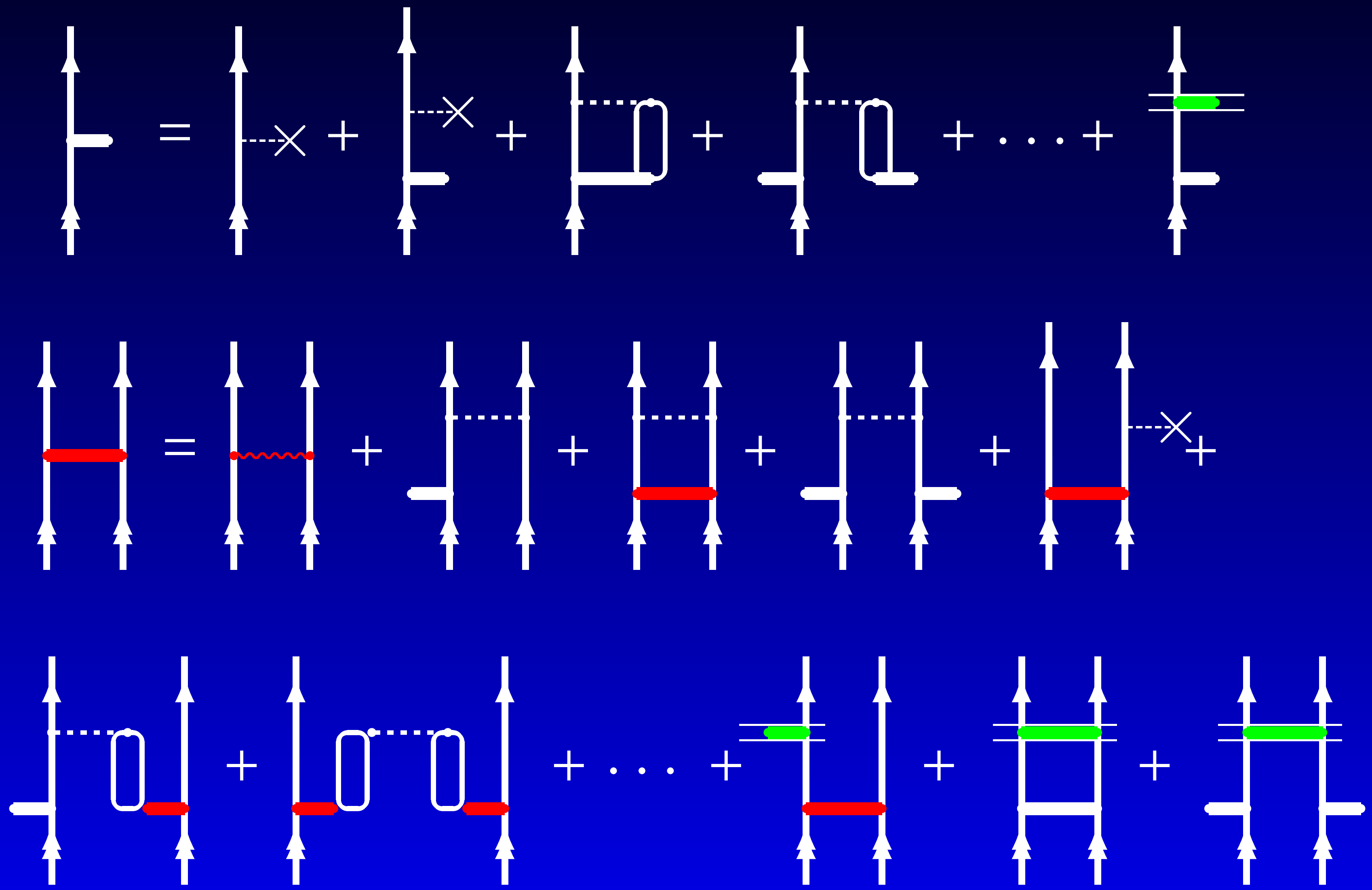
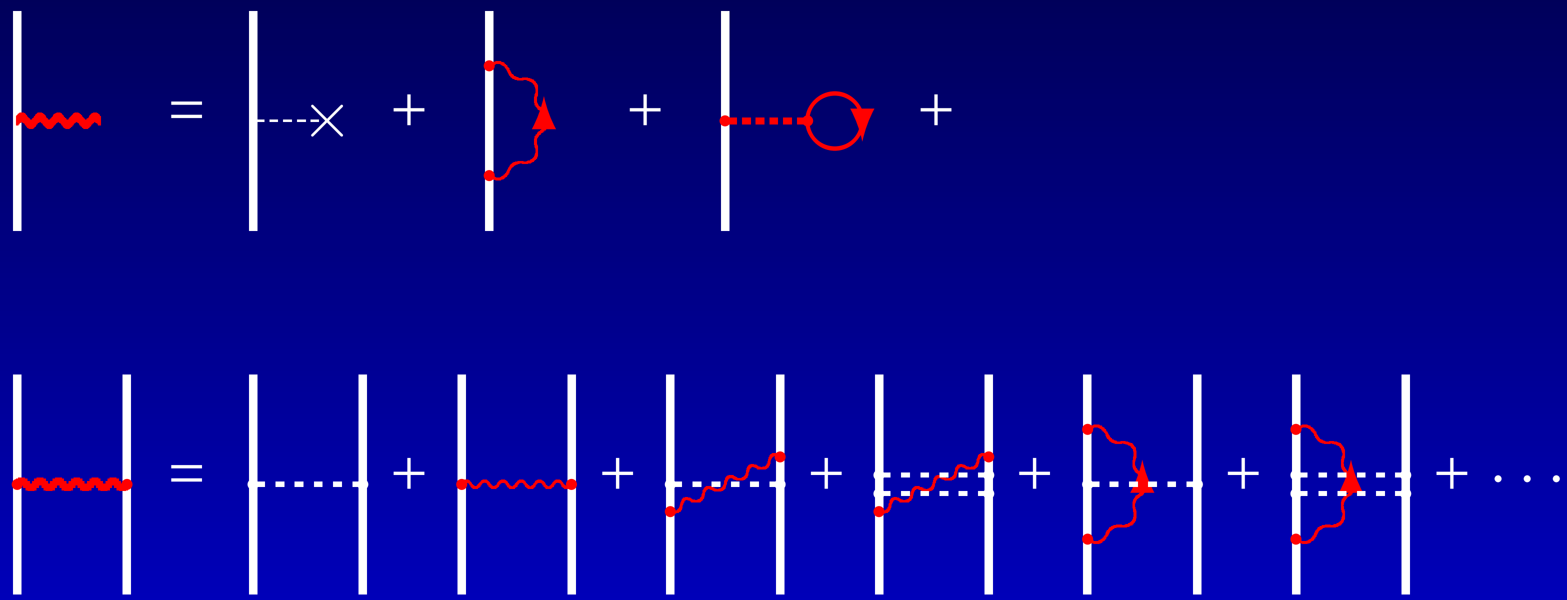
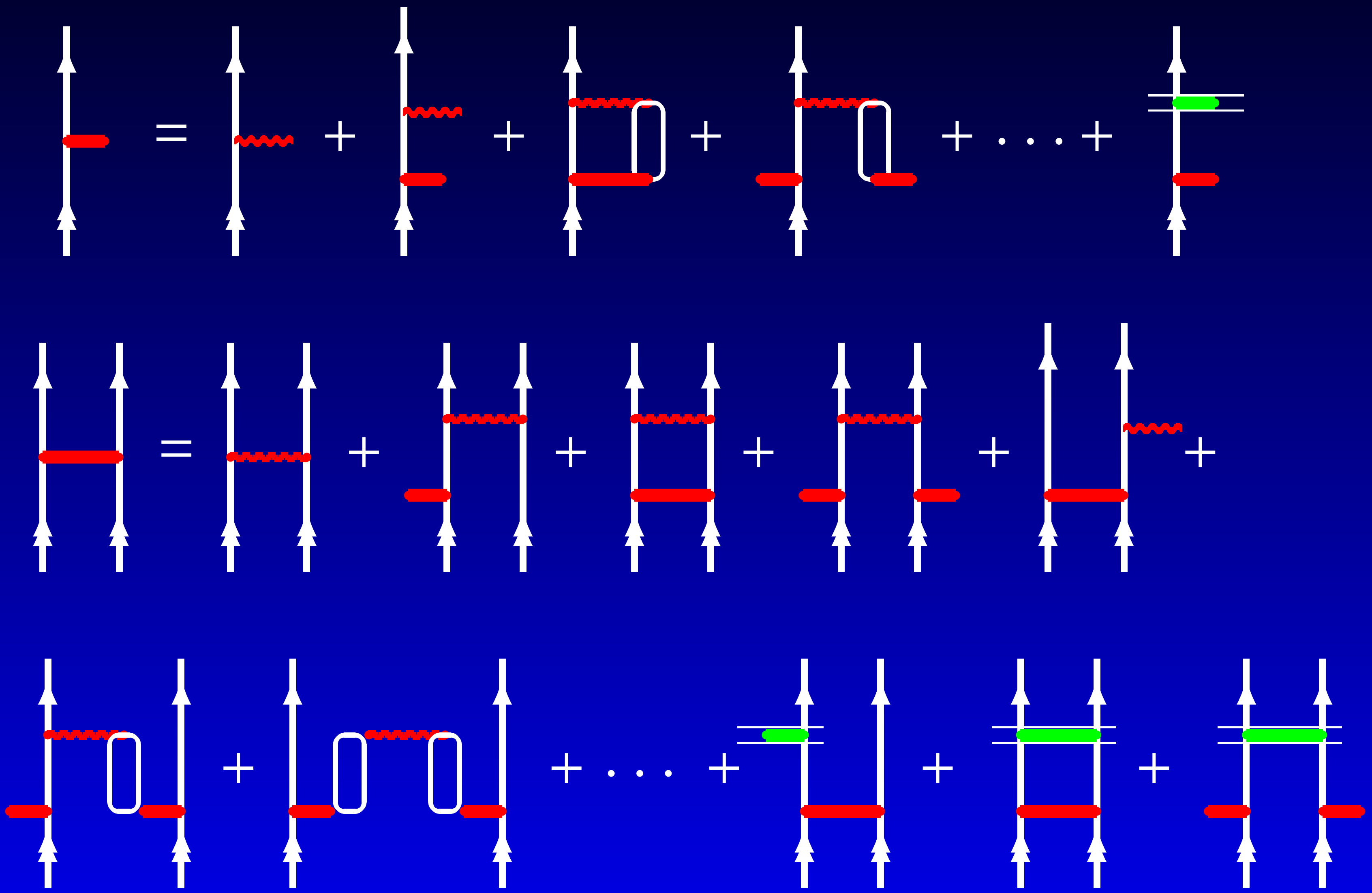


MBPT-QED

QED potentials



Coupled-cluster CCSD(T)



Summary

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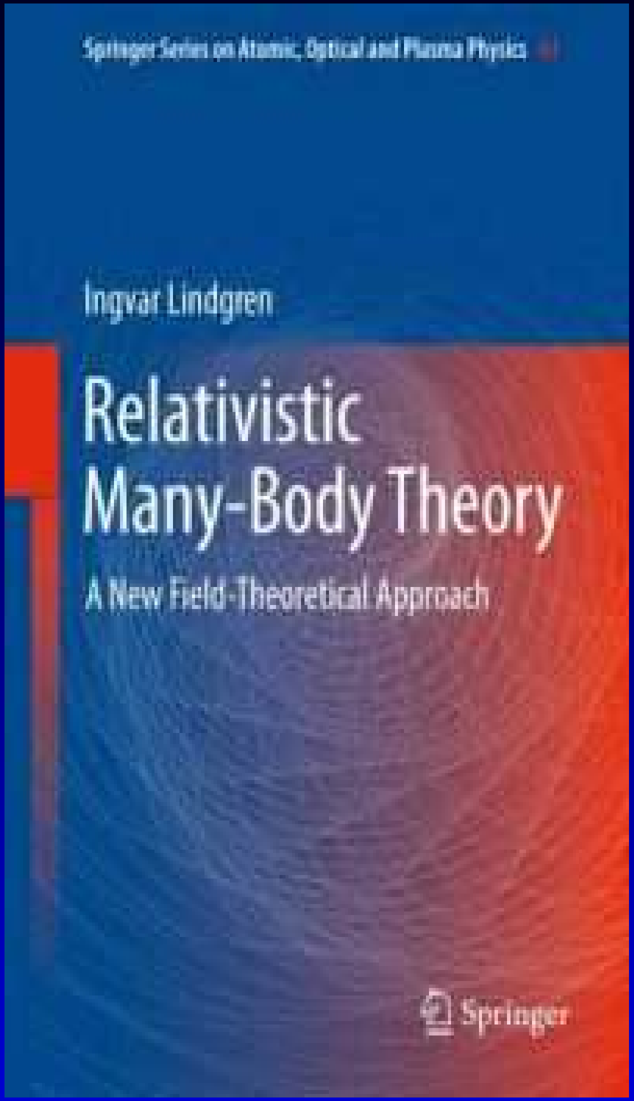
Application to more general systems might be possible by using the coupled-cluster approach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Ingvar Lindgren
Relativistic Many-Body Theory
A New Field-Theoretical Approach
Springer

Coworkers

Sten Salomonson
Daniel Hedendahl
Johan Holmberg

Thank you!