Development of Many-Body Perturbation Theory

How to combine with Quantum ElectroDynamics?

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WHY?
Fundamental problem

Seemingly incompatible
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MBPT is based upon quantum mechanics with a single time

\[ \Psi(t, x_1, x_2...) \]
**Fundamental problem**

Seemingly incompatible

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QED is based on relativistic field theory with individual times

\[ \Psi(t_1 x_1, t_2 x_2, \ldots) \]
**Fundamental problem**

Seemingly incompatible

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Compromise: **Equal-time approximation**
Fundamental problem

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Compromise: Equal-time approximation

Very small effect in atomic/molecular physics
How can QED effects be included in a many-body problem in a systematic fashion?
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For chemical systems the situation is the reversed. Correlated wave function natural starting point
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To treat correlation by QED is highly inefficient. Works for highly charged ions with small correlation relative to QED

For chemical systems the situation is the reversed. Correlated wave function natural starting point

First-order QED effects can be added to the ENERGY OFTEN INSUFFICIENT
To go further, QED effects should be included in the WAVE FUNCTION.
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QED perturbations are time- or energy dependent.
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Requires time/energy-dependent perturbation theory.
To go further, QED effects should be included in the WAVE FUNCTION.

QED perturbations are time- or energy dependent.

Requires time/energy-dependent perturbation theory.

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

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

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

\[ \Psi_0^\alpha = P \Psi^\alpha \quad \text{Intermediate normalization} \]
MBPT Calculations

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

Linked diagram theorem

Graphical representation: Unlinked diagrams cancel

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

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\[ \psi_0^\alpha = P \psi^\alpha \quad \text{Intermediate normalization} \]

Bloch equation \((\text{Bloch 1958, IL 1974})\)

\[ [\Omega, H_0] P = Q \left( V \Omega - \Omega W \right) \text{linked } P \]

\[ -\Omega W \quad \text{Model-space contribution} \]

\[ W = PV \Omega P \quad \text{Effective interaction} \]
Model-space contribution

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

Second order: \( \Omega^{(2)} P_\varepsilon = \Gamma Q (V \Omega^{(1)} - \Omega^{(1)} P_\varepsilon W^{(1)}) P_\varepsilon \)
Model-space contribution

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

Second order : \( \Omega^{(2)} P_\varepsilon = \Gamma Q (V\Omega^{(1)} - \Omega^{(1)} P_\varepsilon' W^{(1)}) P_\varepsilon \)
Model-space contribution

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

Second order: \( \Omega^{(2)} P\xi = \Gamma Q(V\Omega^{(1)} - \Omega^{(1)} P\xi' W^{(1)}) P\xi \)

Unlinked diagrams cancel
Model-space contribution

Remainder: Folded diagrams

\[ \Omega^{(1)}(\varepsilon) - \Omega^{(1)}(\varepsilon') \Rightarrow \text{Folded} \]
Model-space contribution

Remainder: Folded diagrams

\[
\left( \Omega^{(1)}(\mathcal{E}) - \Omega^{(1)}(\mathcal{E}') \right) \frac{P_{\mathcal{E}'} V P_{\mathcal{E}}}{\mathcal{E} - \mathcal{E}'} = \frac{\delta \Omega^{(1)}}{\delta \mathcal{E}} P_{\mathcal{E}'} V P_{\mathcal{E}}
\]
Model-space contribution

Remainder: Folded diagrams

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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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\[
\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)}
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Model-space contribution

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\[
\Omega = \Gamma Q \left[ V \Omega - \Omega W \right]_{\text{linked}}
\]
Relativistic MBPT
(Breit 1931, Brown-Ravenhall 1951, Sucher 1980)
Dirac-Coulomb-Breit Approximation

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

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

Instantaneous Breit interaction
Relativistic MBPT

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

Dirac-Coulomb-Breit Approximation

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Instantaneous Breit interaction

No-(virtual)-pair approximation (NVPA)
QED effects

Effects beyond NVPA - Energy dependent

Order $\alpha^3$ and higher

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

Non-radiative effects  Radiative effects
All-order methods

\[ \Omega = 1 + \Omega_1 + \Omega_2 + \cdots \]
All-order methods

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

\[ \Omega_2 : \quad = \quad + \quad + \quad + \quad + \cdots + \quad \]
All-order methods

\[ \Omega = 1 + \Omega_1 + \Omega_2 + \cdots \]

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

\[ \Omega_2 : \quad \text{Coulomb interaction} \]

\[ \text{Folded} \]

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)

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

All diagrams connected
Coupled-cluster approach

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All diagrams connected

Bloch equation

\[ (E_0 - H_0) T = (V \Omega P - \Omega W)_{\text{conn}} \]
Coupled-cluster approach

Normal-ordered exponential Ansatz

( IL1978, Mukherjee 1995, 97)

Open shells (multiple reference)

\[ \Omega = \{e^T\} = 1 + T + \frac{1}{2}\{T^2\} + \frac{1}{3!}\{T^3\} + \cdots \]

Eliminates spurious contractions between open-shell lines
Coupled-cluster approach

Normal-ordered exponential Ansatz

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\[ \Omega = \{e^T\} = 1 + T + \frac{1}{2}\{T^2\} + \frac{1}{3!}\{T^3\} + \cdots \]

Eliminates spurious contractions between open-shell lines

Bloch equation

\[ [T, H_0] P = Q(V\Omega - \Omega W)_{\text{conn}} \]
Coupled-cluster approach

Open shells

\[ \mathcal{T} = \mathcal{T}_0 + \mathcal{T}_0 \cdot \mathcal{T}_1 + \cdots + \mathcal{T}_n \]

\[ H = H_0 + H_0 \cdot H_1 + H_1 + H_1 \cdot H_2 + H_2 \cdot H_3 + \cdots \]

Folded
Numerical, closed shells

BH$_3$ molecule (Shavitt et al. 1972)

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<th>Total</th>
<th>Connected</th>
<th>Disconnected</th>
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<td>0.1</td>
<td></td>
</tr>
<tr>
<td>Two-body</td>
<td>97.2</td>
<td>97.2</td>
<td>≤ 0.1</td>
</tr>
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<td>Three-body</td>
<td>0.8</td>
<td>0.8</td>
<td>≤ 0.01</td>
</tr>
<tr>
<td>Four-body</td>
<td>1.9</td>
<td>≤ 0.01</td>
<td>1.9</td>
</tr>
</tbody>
</table>
QED Calculations

Standard methods
QED Calculations

Standard methods

a) S-matrix formulation
QED Calculations

Standard methods

a) **S-matrix** formulation

b) Two-times Green’s function developed by Shabaev et al. St. Petersburg
QED Calculations

Standard methods

a) S-matrix formulation

b) Two-times Green’s function
developed by Shabaev et al. St. Petersburg

c) Covariant-evolution operator method
developed by the Gothenburg group
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Standard methods

a) **S-matrix** formulation

b) **Two-times Green’s function**
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All three methods in practice limited to two-photon exchange - only **first-order correlation**. Of no interest to chemists
QED Calculations

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CEO has similar structure as MBPT. Basis for unification
Beyond standard methods
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Standard methods treat **energy-independent** (Coulomb) interactions and **energy-dependent** QED perturbations **separately**
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This leaves out the combination effect.
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Employing time-dependent perturbation theory enables us to combine MBPT and QED.
Beyond standard methods

Standard methods treat energy-independent (Coulomb) interactions and energy-dependent QED perturbations separately.

This leaves out the combination effect.

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)

$$G(t, t_0) = \frac{\langle 0_H | T[\hat{\psi}_H(x)\hat{\psi}^\dagger_H(x_0)] | 0_H \rangle}{\langle 0_H | 0_H \rangle}$$
Time-dependent perturbation theory

Covariant Evolution Operator (CEO)

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The single-particle CEO analogously

$$U_{Cov}(t, t_0) = \int \int d^3x \, d^3x_0 \, \hat{\psi}(x) \langle 0_H | T[\hat{\psi}_H(x)\hat{\psi}^\dagger_H(x_0)] | 0_H \rangle \hat{\psi}(x_0)$$
Time-dependent perturbation theory

Covariant Evolution Operator (CEO)

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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

\[ \Psi_{\text{Rel}}(t) = U_{\text{Cov}}(t, t_0) \Psi_{\text{Rel}}(t_0) \]
Time-dependent perturbation theory

**Green’s operator**

Covariant evolution operator represents the time evolution of relativistic wave function

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

Evolution operator singular due to intermediate model-space states
Time-dependent perturbation theory

Green’s operator

Covariant evolution operator represents the time evolution of relativistic wave function

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

Evolution operator singular due to intermediate model-space states

Regular part known as Green’s operator

$$U_{\text{Cov}}(t, t_0) P = \mathcal{G}(t, t_0) P U_{\text{Cov}}(0, t_0) P$$
Time-dependent perturbation theory

The Green’s operator acts as the time-dependent relativistic wave operator
Time-dependent perturbation theory

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$$\Psi^\alpha(t) = U_{\text{Cov}}(t, t_0) \Psi^\alpha(t_0)$$
Time-dependent perturbation theory

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

\[ \Psi^\alpha(t) = U_{\text{Cov}}(t, -\infty) \Psi^\alpha(-\infty) \]
Time-dependent perturbation theory

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

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

$$U_{\text{Cov}}(t, t_0)P = \mathcal{G}(t, t_0) P U_{\text{Cov}}(0, t_0)P$$
Time-dependent perturbation theory

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

\[
\Psi^{\alpha}(t) = U_{\text{Cov}}(t, -\infty) \Psi^{\alpha}(-\infty)
\]

\[
\Psi^{\alpha}(t) = \mathcal{G}(t, t_0) \left[ PU_{\text{Cov}}(0, t_0) \Psi^{\alpha}(-\infty) \right]
\]
Time-dependent perturbation theory

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

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\[ \Psi^\alpha(t) = \mathcal{G}(t, -\infty) \Psi^\alpha_0 \]
Time-dependent perturbation theory

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

\[ \Psi_\alpha(t) = U_{\text{Cov}}(t, -\infty) \Psi_\alpha(-\infty) \]

\[ \Psi_\alpha(t) = G(t, t_0) \underbrace{PU_{\text{Cov}}(0, t_0)}_{\text{exact}} \Psi_\alpha(-\infty) \]

\[ \Psi_\alpha(t) = G(t, -\infty) \Psi_\alpha^0 \]

Compare std MBPT:

\[ \Psi = \Omega \Psi_0 \]
Time-dependent perturbation theory

Expansion of the Green’s operator

\[ U(t)P_\varepsilon = G(t) P_\varepsilon' U(0) P_\varepsilon \]

\[ G^{(2)}(t) P_\varepsilon = Q \left( G^{(1)}(t) U^{(1)}(0) - G^{(1)}(t) P_\varepsilon' U^{(1)}(0) \right) P_\varepsilon \]
Time-dependent perturbation theory

Expansion of the Green’s operator

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Compare std wave operator

\[ \Omega P = \Gamma_Q \left( V\Omega - \Omega PW \right) P \]

\[ \Omega^{(2)} P_\varepsilon = \Gamma_Q \left( V\Omega^{(1)} - \Omega^{(1)} P_\varepsilon W^{(1)} \right) P_\varepsilon \]
Time-dependent perturbation theory

**Folded diagrams**

\[ \Omega^{(2)} = \Gamma_Q V \Omega^{(1)} + \frac{\delta \Omega^{(1)}}{\delta \epsilon} W^{(1)} = \Gamma_Q V \Omega^{(1)} - \Gamma_Q \Omega^{(1)} W^{(1)} \]

Energy-independent perturbations
Time-dependent perturbation theory

Folded diagrams

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

Energy-independent perturbations

\[ \mathcal{G}^{(2)} = \Gamma_Q V \mathcal{G}^{(1)} - \Gamma_Q \mathcal{G}^{(1)} W^{(1)} + \Gamma_Q \frac{\delta V}{\delta \mathcal{E}} W^{(1)} \]

Energy-dependent perturbations
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Energy-independent perturbations

\[ G^{(2)} = \Gamma_Q V G^{(1)} - \Gamma_Q G^{(1)} W^{(1)} + \Gamma_Q \frac{\delta V}{\delta \mathcal{E}} W^{(1)} \]

Energy-dependent perturbations
Time-dependent perturbation theory

Bloch eqn for time-dependent perturbation theory

\[
[\mathcal{G}, H_0] = V\mathcal{G} - \mathcal{GW} + \left[ \frac{\delta\mathcal{G}}{\delta\epsilon}, H_0 \right] W
\]

* derivation restricted to last interaction
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 \epsilon}, H_0 \right] W
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\[W = PV \Omega P\]
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Compare std MBPT:

\[
[\Omega, H_0] = V\Omega - \Omega W \quad (W = PV\Omega P)
\]
Time-dependent perturbation theory

Bloch eqn for time-dependent perturbation theory

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[\mathcal{G}, H_0] = V\mathcal{G} - \mathcal{G}W + \left[ \frac{\delta*\mathcal{G}}{\delta\varepsilon}, H_0 \right] W
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Compare std MBPT:

\[
[\Omega, H_0] = V\Omega - \Omega W
\]

\( W = PV\Omega P \)

Procedures completely compatible
Time-dependent perturbation theory

How to evaluate the QED effects perturbatively?
Time-dependent perturbation theory

Gell-Mann-Low theorem

\[ H_D |\Psi\rangle = \left( H_0 + V_C + \nu_T \right) |\Psi\rangle = E |\Psi\rangle \]
Time-dependent perturbation theory

Gell-Mann-Low theorem

\[
H_D |\Psi\rangle = \left( H_0 + V_C + \nu_T \right) |\Psi\rangle = E |\Psi\rangle
\]

\[ V = V_C + \nu_T \]

Coulomb + Transverse
Time-dependent perturbation theory

Gell-Mann-Low theorem

\[ H_D |\Psi\rangle = \left( H_0 + V_C + v_T \right) |\Psi\rangle = E |\Psi\rangle \]

\[ V = V_C + v_T \]

Coulomb + Transverse

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

\[ v_T = - \int d^3x \hat{\psi}(x)\hat{\psi}(x) e^a A_\mu(x) A_\nu(x) \]

Slides with Prosper/LATeX – p. 30/55
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

\[
\langle rs|\mathcal{V}_{sp}(\mathcal{E})|tu\rangle = \langle rs\right| \int_0^\infty d\kappa f(\kappa) \frac{1}{\mathcal{E} - \varepsilon_r - \varepsilon_u - \kappa} |tu\rangle
\]

\[
f(\kappa) = \sum_l V^l(\kappa r_1) \cdot V^l(\kappa r_2)
\]
Time-dependent perturbation theory

Single-photon exchange requires two perturbations

\[ \langle rs | V_{sp}(E) | tu \rangle = \langle rs | \int_0^\infty d\kappa \frac{1}{E - \varepsilon_r - \varepsilon_u - \kappa} f(\kappa) | tu \rangle \]

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\[ f(\kappa) = \sum_l V^l(\kappa r_1) \cdot V^l(\kappa r_2) \]

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

\[ H_D |\Psi_l\rangle = \left( H_0 + V_C + V^l \right) |\Psi_l\rangle = E |\Psi_l\rangle \]
Time-dependent perturbation theory

Iteration of time-independent perturbations
Time-dependent perturbation theory

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Iteration of time-independent perturbations
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.
Self-energy regularization

Dimensional regularization in Coulomb gauge most appropriate to use in MBPT/QED
Never used before.

\[
\begin{align*}
\begin{array}{c}
\includegraphics[width=0.5\textwidth]{diagram.png}
\end{array}
\end{align*}
\]

Zero- and one-pot. terms evaluated using Adkins formulas
Modified by J. Holmberg, PRA\textbf{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

<table>
<thead>
<tr>
<th>Z</th>
<th>Coulomb gauge</th>
<th>Feynman gauge</th>
</tr>
</thead>
<tbody>
<tr>
<td>18</td>
<td>1.216901(3)</td>
<td>1.21690(1)</td>
</tr>
<tr>
<td>54</td>
<td>50.99727(2)</td>
<td>50.99731(8)</td>
</tr>
<tr>
<td>66</td>
<td>102.47119(3)</td>
<td>102.4713(1)</td>
</tr>
<tr>
<td>92</td>
<td>355.0430(1)</td>
<td>355.0432(2)</td>
</tr>
</tbody>
</table>

Self-energy

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

\[ \frac{\delta \Sigma}{\delta \mathcal{E}} = \Lambda_0 \]
Self-energy

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Singularity cancelled by vertex correction due to Ward identity

\[ \frac{\delta \Sigma}{\delta \mathcal{E}} = \Lambda_0 \]

Both are charge divergent and have to be renormalized
Time-dependent perturbation theory

Iteration of time-dependent perturbations

QED Pair function
Time-dependent perturbation theory

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Iteration of time-dependent perturbations

QED Pair function

\[
H \quad = \quad \text{QED Pair function}
\]
## Numerical illustration

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

<table>
<thead>
<tr>
<th>Z</th>
<th>Two-photon</th>
<th>Combined QED-correlation BEYOND two-photon</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>0.0033</td>
<td>0.0072</td>
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<tr>
<td>14</td>
<td>0.0080</td>
<td>0.0101</td>
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<tr>
<td>18</td>
<td>0.0150</td>
<td>0.0154</td>
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<tr>
<td>24</td>
<td>0.0305</td>
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<tr>
<td>30</td>
<td>0.052</td>
<td>0.0244</td>
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<tr>
<td>42</td>
<td>0.112</td>
<td>0.0286</td>
</tr>
<tr>
<td>50</td>
<td>0.0320</td>
<td>0.0400</td>
</tr>
<tr>
<td>66</td>
<td></td>
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</tr>
</tbody>
</table>
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Might have the potential, since the standard and QED procedures are completely compatible.
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QED effects need only be inserted to the degree that is relevant.
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CCSD(T)
Can this be applied to larger systems???

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QED effects need only be be inserted to the degree that is relevant

CCSD(T)
H = \text{Diagram}
Coupled-cluster CCSD

\[ T = T \times + T \times + T P + T + \cdots + T \]

\[ H = H + H + H + H + H + H \]

\[ \cdots \]

\[ H + H + H + H \]
Coupled-cluster CCSD

\[ T = \int \times + \int \times + \int \text{P} + \int \text{H} + \cdots + \int \text{H} \]

\[ \text{H} = \int \text{H} + \int \text{H} + \int \text{H} + \int \text{H} + \int \text{H} + \int \text{H} \]

\[ \text{H} = \int \text{H} + \int \text{H} + \int \text{H} + \int \text{H} + \int \text{H} + \int \text{H} \]

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MBPT-QED

QED potentials

\[ \text{potentials} = \text{potentials} + \text{potentials} + \text{potentials} \]
Coupled-cluster CCSD(T)
Summary

A procedure has been developed for combining MBPT and QED, based upon the covariant-evolution operator method.
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Application to more general systems might be possible by using the coupled-cluster approach.
Coworkers

Sten Salomonson
Daniel Hedendahl
Johan Holmberg
Thank you!