Theor Chem Acc (2015) 134:123
DOI 10.1007/s00214-015-1707-6

REGULAR ARTICLE

# Combination of many-body perturbation theory and quantum electrodynamics

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Received: 22 May 2015 / Accepted: 25 July 2015 / Published online: 6 October 2015


**Abstract** A procedure for energy-dependent perturbation expansion has been developed, based upon the covariant evolution operator method. This makes it possible to treat energy-dependent perturbations very much like the energy-independent ones in standard many-body perturbation theory. This has been applied to the non-radiative QED perturbations (retardation and virtual electron–positron pairs) as well as the radiative ones (electron self-energy, vacuum polarization and vertex correction). The combination of QED and electron correlation, beyond two-photon exchange, has been evaluated, using the Coulomb gauge. It turned out that in that gauge the extremely time-consuming model-space contributions of the self-energy and vertex corrections do not have to be evaluated in full. In the Feynman gauge no sensible results could be obtained in this way, as is demonstrated by the numerical results.

**Keywords** Perturbation theory · Quantum electrodynamics · Electron correlation · Electron self-energy · Green's operator · Covariant evolution operator

Published as part of the special collection of articles "Festschrift in honour of P. R. Surjan".

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## 1 Introduction

The procedures for many-body perturbation calculations (MBPT) for atomic and molecular systems are nowadays very well developed, and the dominating electrostatic as well as magnetic perturbations can be taken to essentially all orders of perturbation theory (see, for instance, [1]). Less pronounced, but in many cases still quite significant, are the quantum electrodynamical (QED) perturbations—retardation, virtual pairs, electron self-energy, vacuum polarization and vertex correction. Sophisticated procedures for their evaluation have also been developed, but for practical reasons such calculations are prohibitive beyond second order (two-photon exchange). Pure QED effects beyond that level can be expected to be very small, but the *combination* of QED and electrostatic perturbations (electron correlation) can be significant. However, none of the previously existing methods for MBPT or QED calculations is suited for this type of calculation.

We have during the past decade developed an energy-dependent perturbation procedure, based on a "*covariant evolution operator method*" [2–5], that will make it possible to handle energy-dependent QED perturbations very much in the same way as the energy-independent ones in MBPT.

## 2 Covariant evolution operator

The time-evolution operator for the Schrödinger wave function transforms the wave function from one time to another

$$\Psi(t) = U(t, t_0)\Psi(t_0). \tag{1}$$

In the *interaction picture* the wave function has the time dependence

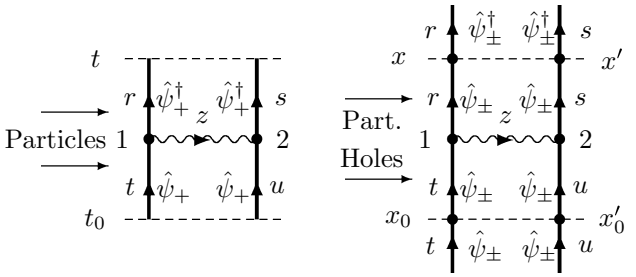


**Fig. 1** Comparison between the standard evolution operator and the covariant evolution operator for single-photon exchange in the equal-time approximation

$$\Psi(t) = \mathrm{e}^{-it(E-H_0)/\hbar}\Psi(0) \tag{2}$$

with the Hamiltonian in the *Schrödinger representation* $H = H_0 + V$ and $E$ being the exact energy of the state. An equation for the evolution operator follows from the time-dependent Schrödinger equation.

The non-relativistic evolution operator is in first order represented by the first Feynman diagram in Fig. 1. It is non-covariant, since time flows only in the positive direction. If we insert electron propagators in the in- and outgoing orbital lines, time can flow in both directions, and we get a covariant form of the evolution operator, represented by the second diagram.

The *covariant evolution operator* for a ladder of retarded interactions between the electrons is given by

$$U(t,-\infty)\,P_{\mathcal{E}} = \mathrm{e}^{-it(\mathcal{E}-H_0)}[1 + \Gamma(\mathcal{E})\,V(\mathcal{E}) + \Gamma(\mathcal{E})\,V(\mathcal{E})\,\Gamma(\mathcal{E})\,V(\mathcal{E}) + \cdots]P_{\mathcal{E}}, \tag{3}$$

assuming that we have a small damping factor on the perturbation so that $t = -\infty$ corresponds to an unperturbed state. Here, $P_{\mathcal{E}}$ is the projection operator for the part of the model space of energy $\mathcal{E}$. $\Gamma(\mathcal{E})$ is the resolvent

$$\Gamma(\mathcal{E}) = \frac{1}{\mathcal{E} - H_0}.$$

The evolution operator is (quasi)singular, when an intermediate or final state lies in the model space.

The evolution operator without intermediate model-space states is

$$U_0(t,-\infty)\,P_{\mathcal{E}} = \mathrm{e}^{-it(\mathcal{E}-H_0)}[1 + \Gamma_Q(\mathcal{E})\,V(\mathcal{E}) + \Gamma_Q(\mathcal{E})\,V(\mathcal{E})\,\Gamma_Q(\mathcal{E})\,V(\mathcal{E}) + \cdots]P_{\mathcal{E}}, \tag{4}$$

which is regular. Here, $\Gamma_Q$ is the reduced resolvent

$$\Gamma_Q = \frac{Q}{\mathcal{E} - H_0}.$$

and $Q$ is the projection operator for the space outside the model space.

We define a *Green's operator* by

$$U(t,-\infty)P = \mathcal{G}(t,-\infty)\cdot PU(0,-\infty)P, \tag{5}$$

which is free from singularities and analogous to the Green's function in field theory. In the definition the heavy dot indicates that the Green's operator acts on the intermediate model-space state. The evolution operator and the Green's operator depend on the energy of the model-space states they are operating on. We then write the relation

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

leaving out the initial time $t_0 = -\infty$ and assuming that the model-space energies might be slightly different.

The definition leads to *counterterms*, which form *model-space contributions* (MSC) that eliminate the singularities so that the Green's operator becomes regular for all times.

The Green's operator transforms the unperturbed state in the model space, $\Psi_0$, to the corresponding exact (target) state, $\Psi(t)$, at a given time $t$

$$\Psi(t) = \mathcal{G}(t,\mathcal{E})\Psi_0(\mathcal{E}) \tag{6}$$

and hence acts as a time-dependent wave operator. For $t = 0$ it is the energy-dependent analogue of the standard wave operator in standard MBPT [1]

$$\Omega(\mathcal{E}) = \mathcal{G}(0,\mathcal{E}). \tag{7}$$

### 2.1 Model-space contributions

Including the counterterm, the first-order Green's operator becomes

$$\mathcal{G}^{(1)}(t,\mathcal{E})P_{\mathcal{E}} = \mathcal{G}^{(0)}(t,\mathcal{E})\,U^{(1)}(0,\mathcal{E})P_{\mathcal{E}} - \mathcal{G}^{(0)}(t,\mathcal{E}')P_{\mathcal{E}'}U^{(1)}(0,\mathcal{E})P_{\mathcal{E}}, \tag{8}$$

where we observe that the Green's operator in the counterterm has the energy parameter $\mathcal{E}'$. Here,

$$\mathcal{G}^{(0)}(t,\mathcal{E}) = \mathrm{e}^{-it(\mathcal{E}-H_0)} \tag{9}$$

is the zeroth-order Green's operator.

When there is an intermediate model-space state $P_{\mathcal{E}'}$ in the first term, we have a MSC given by

$$\begin{aligned}\Big[\mathcal{G}^{(0)}(t,\mathcal{E}) - \mathcal{G}^{(0)}(t,\mathcal{E}')\Big]P_{\mathcal{E}'}U^{(1)}(0,\mathcal{E})P_{\mathcal{E}} &= \Big[\mathcal{G}^{(0)}(t,\mathcal{E}) - \mathcal{G}^{(0)}(t,\mathcal{E}')\Big]P_{\mathcal{E}'}\frac{V(\mathcal{E})}{\mathcal{E}-\mathcal{E}'}P_{\mathcal{E}} \\ &= \frac{\delta\mathcal{G}^{(0)}(t,\mathcal{E})}{\delta\mathcal{E}}\,P_{\mathcal{E}'}V(\mathcal{E})P_{\mathcal{E}}.\end{aligned} \tag{10}$$

In the case of exact degeneracy, the difference ratio goes over into a partial derivative. The complete first-order Green's operator then becomes

$$\mathcal{G}^{(1)}(t,\mathcal{E})P_{\mathcal{E}} = \mathcal{G}^{(0)}(t,\mathcal{E})\Gamma_Q V P_{\mathcal{E}} + \frac{\delta\mathcal{G}^{(0)}(t,\mathcal{E})}{\delta\mathcal{E}} P_{\mathcal{E}'} V(\mathcal{E}) P_{\mathcal{E}}, \tag{11}$$

where the second term is the MSC.

The *effective interaction* that gives rise to the energy shift is given by

$$W = P\left(i\frac{\partial}{\partial t}\mathcal{G}(t,-\infty)\right)_{t=0} P, \tag{12}$$

and applied to the first-order Green's operator we find that the first-order effective interaction is as expected

$$W^{(1)} = PVP. \tag{13}$$

Continuing this process we find that the second-order Green's operator becomes

$$\mathcal{G}^{(2)}(t,\mathcal{E})P_{\mathcal{E}} = \Gamma_Q V_2 \Gamma_Q V_1 + \frac{\delta\Gamma_Q V_2}{\delta\mathcal{E}} P V_1 P, \tag{14}$$

where we have assumed that the interactions might be different. If the interactions are energy independent, this goes over into the second-order wave operator of standard MBPT [1]

$$\Omega^{(2)} = \Gamma_Q V_2 \Gamma_Q V_1 - \Gamma_Q \Omega^{(1)} W^{(1)}. \tag{15}$$

The second-order effective interaction becomes

$$W^{(2)} = P V_2 \Gamma_Q V_1 + P\frac{\delta V_2}{\delta\mathcal{E}} P V_1 P. \tag{16}$$

The last terms in Eqs. (14) and (16) are MSC.

The Green's operator satisfies a Bloch-like equation

$$\mathcal{G} = \mathcal{G}^{(0)} + \Gamma_Q V \mathcal{G} + \frac{\delta^*\mathcal{G}}{\delta\mathcal{E}} W, \tag{17}$$

where the asterisk represents derivation with respect to the last interaction $\Gamma_Q V$ and with respect to $\mathcal{G}^{(0)}$ when no factor of $\Gamma_Q V$ is present. When the interactions are energy independent, this equation goes over into the Bloch equation in standard MBPT [1, 6, 7].

## 3 Application to Helium-like ions

The procedure sketched above has recently been applied to the ground state of medium-heavy helium-like ions. We have evaluated the effect of QED combined with electron correlation, defined as the interaction with at least two Coulomb interactions. The QED part is here restricted to first order and consists of "non-radiative" effects (retardation of the electromagnetic interaction and effect of virtual electron–positron pairs) as well as "radiative" effects (electron self-energy, vacuum polarization and vertex correction).

It is true that in this procedure we miss some second-order QED effects which can be evaluated by standard QED methods. To mix these in a general way with electron correlation is beyond reach for the moment. We have found, however, that higher-order correlation is considerably more important than second-order QED effects for medium-heavy elements. Therefore, this procedure does include the most important effects of many-body QED in the cases studied.

The effect of retardation in combination with electron correlation was evaluated by Daniel Hedendahl in his PhD thesis [8], including the effect of crossing Coulomb interaction and the effect of virtual pairs. The effect was found to be of the order of 5–10 meV for the ground state of helium-like ions in the range $Z = 20$–$40$. This is one order of magnitude smaller than the corresponding two-photon effect.

To evaluate the corresponding radiative effects is considerably more difficult. First or all, these effects are divergent and the effects have to be regularized and renormalized, which has to be done in a covariant way. Several schemes for this procedure exist, but the most effective scheme is the dimensional regularization, where the calculations are performed in $(4-\epsilon)$ dimensions, $\epsilon$ being a small positive number. Then all integrals are finite, and finally the limit $\epsilon \to 0$ is taken.

All calculations of radiative QED effects have until very recently been performed using the Feynman gauge. The procedure for dimensional regularization was developed for that gauge around 1990 mainly by Snyderman at Livermore Nat. Lab. [10], and the procedure has been applied by several laboratories [11, 12]. We have demonstrated that it is more advantageous to use the Coulomb gauge in combination with electron correlation. Here, the dimensional regularization is more complicated, but a working procedure was developed a few years ago by Hedendahl and Holmberg [9] at our laboratory, based upon the work of Adkins [13, 14]. This procedure was tested for hydrogen-like ions, and the result is given in Table 1, showing the results in terms of the $F(Z\alpha)$ function,

$$\Delta E^{SE} = \frac{\alpha}{\pi}(Z\alpha)^4 mc^3 F(Z\alpha), \tag{18}$$

**Table 1** Values of the function $F(Z\alpha)$ in Eq. (18) for the self-energy of the ground state of hydrogen-like ions (from Hedendahl and Holmberg [9])

| $Z$ | Coulomb gauge | Feynman auge |
|---|---|---|
| 18 | 3.444 043(9) | 3.444 04(3) |
| 26 | 2.783 762(3) | 2.783 77(1) |
| 36 | 2.279 314(2) | 2.279 316(7) |
| 54 | 1.181 866 2(6) | 1.781 868(3) |
| 66 | 1.604 461 5(4) | 1.604 462(2) |
| 82 | 1.487 258 4(4) | 1.487 259(1) |
| 92 | 1.472 424 1(4) | 1.472 425(1) |

**Table 2** Two-photon electron self-energy and vertex correction for the ground state of He-like argon ion, using the Coulomb and Feynman gauges, from Holmberg et al. [5] (in meV)

| Gauge | Wave function contr. | | MSC | VTX | MCS,VTX | Total SE |
|---|---|---|---|---|---|---|
| | Zero-pot. | Beyond | Zero-pot | Zero-pot | Beyond | |
| Coulomb | −115.8(7) | 11.55(1) | −24.8(1) | 16.2(1) | −1.1(1) | −113.8(8) |
| Feynman | 1620.8(6) | −1707.7(1) | 3819.0(1) | −3653.3(1) | −192.2(6) | −113(1) |

$Z$ being the nuclear charge and $\alpha$ the fine-structure constant. The gauge invariance is here clearly demonstrated, and it is interesting to note that the accuracy is actually higher in the Coulomb gauge, the reason being that in the Feynman gauge there are large cancellations between different contributions, making the result less accurate.

Very recently these calculations have been extended to helium-like systems by Holmberg et al. [5]. Complete two-photon calculations have been performed in the Coulomb as well as the Feynman gauge, again demonstrating the gauge invariance. It is very striking to observe how different the various contributions behave in the two gauges, as shown in Table 2 for $Z = 18$. In the Coulomb gauge one can see that the wave function contribution dominates and the remaining model-space (MSC) and vertex (VTX) contributions are considerably smaller. In the Coulomb gauge this is not at all the case. Here all contributions are of the same order. In the Coulomb gauge the MSC and VTX beyond zero-potential represent about one per cent of the total effect, while in the Feynman gauge it represents about 200 %. This will have important consequences in higher orders.

The evaluation of the full MSC and VTX correction in combination with electron correlation (beyond second order) is prohibitive in any gauge for computational reason. Fortunately, however, one can conclude from the second-order results that these contributions should be relatively small in the Coulomb gauge and be well approximated by the zero-potential part. This gives the result shown in Table 3 for He-like argon (Z = 18). It is obvious from the results in the table that no sensible results can be deduced by using this approximation in the Feynman gauge.

**Table 3** Correlation effect beyond two-photon exchange for the electron self-energy and vertex correction for the ground state of He-like argon ion, using the Coulomb and Feynman gauges, from Holmberg et al. [5] (in meV)

| Gauge | Wave function contr. | | MSC | VTX | Total SE |
|---|---|---|---|---|---|
| | Zero-pot. | Beyond | Zero-pot | Zero-pot | |
| Coulomb | 4.8 | −0.5 | 1.2 | −0.7 | 4.6 |
| Feynman | −142 | 71 | −24 | 54 | |

## 4 Summary and conclusions

Quite extensive calculations on helium-like ions on the two-photon level have been performed by Artemyev et al., using the Two-Time Green's function [15], and related calculations have been performed by Plante et al., using the relativistic MBPT with first-order QED energy corrections to the energy [16]. The calculations of Artemyev et al. leave out effects beyond second order and those of Plante et al. include them in a very restricted way. We have for the first time performed calculations of combined QED-correlation effects *beyond* the two-photon level on the ground states of a number of helium-like ions, using the recently developed Green's operator method.

The X-ray transition energies of type $1s$–$2p$ for helium-like ions can in many cases be measured with high accuracy, and this can be used to test various computational results and possibly also the QED theory itself.

The agreement between the experiments results and the theoretical results of Artemyev et al. and Plante et al. is in most cases quite good. Nevertheless, Chantler et al. have in a series of papers claimed that there are significant discrepancies between theory and experiments in a number of cases [17, 18]—up to the order of 100 meV. We have found in our calculations that the effects beyond second order for the ground states of medium-heavy ions are only of the order of a few meV (the effect on the excited state should be even smaller), thus considerably smaller than the effects that Chantler et al. claim to have found. Therefore, if these discrepancies are real, they must have other causes than higher-order QED effects.

The findings of Chantler have recently been challenged by Kubiček et al. [19], who found excellent agreement between their experiments and the above-mentioned theoretical calculations. Our numerical results are consequently quite consistent with those of Kubiček et al.

The effect of interactions beyond two-photon exchange has been estimated in a crude way in the publication by Artemyev et al. [15]. We have found that these estimations agree roughly with our accurate calculations for light elements, while there is significant disagreement for heavier elements [5].

In some cases the X-ray energies can be measured with extreme accuracy, and in such cases effects beyond second

order might be relevant. Here the comparison between theory and experiment can be carried out on a higher level in order to find out whether there are effects that cannot be accounted for.

The Green's operator procedure was primarily developed for investigating *static* problems, but it has recently been demonstrated that also *dynamical* processes, such as scattering processes or transitions between atomic states, are governed by the Green's operator and can be handled by a similar procedure [20].

**Acknowledgments** The authors want to congratulate Peter Surjan to his 60th birthday, and I.L. wants in particular to thank Peter for his hospitality during several visits to Budapest. This work has been financially supported by the Helmholtz Association and the Gesellschaft für Schwerionenforschung under the project VH-NG-421.

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