Combining Quantum Electrodynamics and electron correlation

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Abstract

There is presently a large interest in studying highly charged ions in order to investigate the effects of quantum-electrodynamics (QED) at very strong fields. Such experiments can be performed at large accelerators, like that at GSI in Darmstadt, where the big FAIR facility is under construction. Accurate experiments on light and medium-heavy ions can also be performed by means of laser and X-ray spectroscopy. To obtain valuable information, accurate theoretical results are required to compare with.

The most accurate procedures presently used for calculations on simple atomic systems are (i) all-order many-body perturbative expansion with added first-order analytical QED energy corrections, and (ii) two-photon QED calculations. These methods have the shortcoming that the combination of QED and correlational effects (beyond lowest order) is completely missing.

We have developed a third procedure, which can remedy this shortcoming. Here, the energy-dependent QED effects are included directly into the atomic wave function, which is possible with the procedure that we have recently developed.

The calculations are performed using the Coulomb gauge, which is most appropriate for the combined effect. Since QED effects, like the Lamb shift, have never been calculated in that gauge, this has required some development. This is now being implemented in our computational procedure, and some numerical results are presented.

1 Introduction

Highly charged ions are frequently used to investigate QED effects at strong-fields, for instance at the GSI facility at Darmstadt, where H-, He-, Li-, and Be-like ions up to uranium can be produced.

If theory is trusted, comparison between theory and experiment can yield information about nuclear structure, fundamental constants, etc. One example is the proton radius, where the established value, 0.8775(51) fm, is obtained from electron-scattering data and by comparing theory and experiment for atomic hydrogen [1]. (Recently, new measurements on

Table 1: Theoretical value of the electronic g-factor of C^{5+}

Dirac theory	1.998 721 354 39(1)
QED	0.002 320 235 79(3)
Total theory	2.001 041 590 18(3)

Table 2: Transition $1s2s\,^1S_0 - 1s2p\,^3P_1$ in He-like Si (cm^{-1}) (1eV$\approx$ 8000 cm^{-1})

		Reference
Expt'l	7230.585(6)	Myers et al. [5]
RMBPT	7231	Plante et al. [6]
QED	7229(2)	Artemyev et al. [7]

muonic hydrogen have yielded a significantly smaller value, 0.8409(4) [2], and the reason for this discrepancy is presently not understood.)

Another example is the measurement of the electronic g-factor of hydrogen-like ions (see Table 1), which can be determined with high precision by means of a single-ion trap [3]. From this comparison the value of the electron mass was deduced, 0.000 548 579 909 3(3) atomic mass units, which was four times more accurate than the previously accepted value [4].

One question that can be raised here is, of course, to what extent QED can be trusted? Is there a limit, and, if so, what is causing it? Accurate tests of QED can help answering these fundamental questions.

Besides heavy-ion experiments, interesting results can also be achieved by means of laser and X-ray spectroscopy. Some experimental data can be much more accurate than corresponding theoretical evaluations (se Table 2). Here, there is a great challenge to try to improve on the theoretical results.

In Table 3 we compare some X-ray date with accurate theoretical calculations for some medium-heavy helium like ions. The experimental values are taken from ref. [7]. Here, we see that significant deviations can appear.

An interesting question is here how the accuracy of the theoretical calculations could be improved? For most atomic and molecular systems the electron correlation is the dominating perturbation. Therefore, a natural starting point is a procedure where this effect is treated to high order. The standard procedure is then to add first-order QED effects to the *energy*. In

Table 3: Transition $1s^2\,^1S_0 \rightarrow 1s2p\,^1P_1$ in He-like ions (eV)

Z	Artemyev [7]	Plante [6]	Experimental
18	3139.582	3139.580	3139.553(38)
22	4749.644(1)	4749.639	4749.85(7)
36	13026.117(4)	13026.044	13026.8(3)

many cases this procedure yields sufficiently accurate results [6]. In order to reach beyond that level, however, it is necessary to include the QED perturbations into the *wave function*. Since most QED effects are *time or energy dependent*, this requires a time/energy-dependent perturbation procedure.

An alternative procedure that is also frequently used is the two-photon QED procedure, which in many cases leads to quite accurate results [7]. It has the disadvantage, however, that the electron correlation is included only to lowest order.

We have developed a procedure based upon a perturbation expansion, where the electron correlation is essentially carried to all orders and with QED corrections included in the wave function - a procedure that is presently being implemented. We believe this has the potential of yielding higher accuracy than methods presently employed. Before describing this procedure, we shall as a background review the standard time-independent methods.

2 Time-independent Methods for Atomic Calculations

2.1 Non-QED methods

2.1.1 Standard Many-Body Perturbation Theory (MBPT)

We consider a number of "*target states*", satisfying the Schrödinger equation [8]

$$H\Psi^\alpha = E^\alpha \Psi^\alpha \quad (\alpha = 1 \cdots d). \tag{1}$$

For each target state there exists a *model state*, which in intermediate normalization is the projection on the model space

$$\Psi_0^\alpha = P\Psi^\alpha \quad (\alpha = 1 \cdots d). \tag{2}$$

A *wave operator* transforms the model states to the full target states

$$\Psi^\alpha = \Omega\Psi_0^\alpha \quad (\alpha = 1 \cdots d). \tag{3}$$

An *effective Hamiltonian* can be defined, so that it generates the exact energies, operating on the model functions

$$H_{\text{eff}}\Psi_0^\alpha = PH\Omega\Psi_0^\alpha = E^\alpha\Psi_0^\alpha. \tag{4}$$

The Hamiltonian is partitioned into a model Hamiltonian and a perturbation

$$H = H_0 + V. \tag{5}$$

The wave operator satisfies a *Bloch equation*

$$\big[\Omega, H_0\big]P = Q\big[V\Omega - \Omega W\big]_{\text{linked}}P, \tag{6}$$

where the subscript "linked" indicates that - under certain general conditions - only *linked* diagrams contribute (linked-diagram theorem). Here,

$$W = PV\Omega P \tag{7}$$

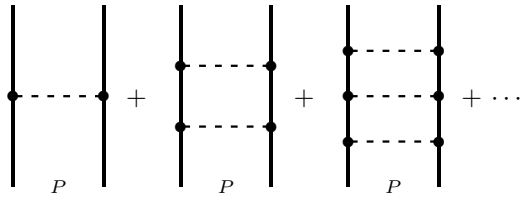

Figure 1: Expanding the two-body part of the wave operator (without singles) leads to the *pair function*.

is the "effective interaction".

The last term of the Bloch equation represents the *model-space contribution*, which is the remainder after the singularities due to intermediate model-space states are eliminated. We shall see that this effect will play an important role in the generalization to energy-dependent formalism that we shall consider below.

2.1.2 All-order methods

In the perturbation expansion certain effects, such as the pair correlation, can be included iteratively to arbitrary order by separating the wave operator by means of second quantization into one-body, two-body ... effects

$$\Omega = \Omega_1 + \Omega_2 + \cdots \tag{8}$$

This leads to the coupled equations

$$\big[\Omega_n, H_0\big]P = Q\big[V\Omega - \Omega W\big]_{\text{linked},n}P. \tag{9}$$

Expanding the two-body part (without singles) leads to the pair function, illustrated in Fig. 1.

By means of the *exponential Ansatz* this leads to the *Coupled-Cluster Approach* [9].

2.1.3 Multi-Configuration Hartree/Dirac-Fock (MCHF/MCDF)

An alternative to the perturbation expansion is the *Multi-Configuration Hartree/Dirac-Fock Method*, where also electron correlation can be included essentially to all orders [10]. In neither scheme QED effects are included, but first-order QED effects can be added to the energy.

2.1.4 Relativistic MBPT

The standard relativistic MBPT is based upon the *Dirac-Coulomb-Breit Approximation* [11]

$$H = \Lambda_+\Big[\sum_{i=1}^{N} h_D(i) + \sum_{i<j}^{N}\frac{e^2}{4\pi r_{ij}} + H_B\Big]\Lambda_+, \tag{10}$$

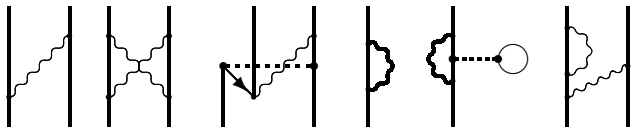

Figure 2: Examples of QED effects.

$$H_B = -\frac{e^2}{8\pi}\sum_{i<j}\Big[\frac{\alpha_i\cdot\alpha_j}{r_{ij}} + \frac{(\alpha_i\cdot r_{ij})(\alpha_j\cdot r_{ij})}{r_{ij}^3}\Big], \tag{11}$$

where the projection operators Λ_+ eliminate negative energy states. This is known as the *No-(Virtual)-Pair Approximation (NVPA)*.

2.1.5 QED effects

The effects beyond NVPA are defined as the *QED corrections*, which are of the order α^3 or higher. They can be separated into (see Fig. 2)

- Non-radiative effects (retardation, virtual pairs)
- Radiative effects (Lamb shift etc.).

2.2 QED methods

There exist several standard methods for QED calculations, the most frequently used methods are

- *S-matrix formulation* [12],
- *Two-times Green's function*, developed by Shabaev et al. at St. Petersburg [13],
- *Covariant-evolution operator method*, developed by the Gothenburg group [14].

All three methods are in practice limited to two-photon exchange, which implies that the electron correlation is treated only to lowest order.

3 Time-dependent perturbation theory: Unification of QED and MBPT

We shall now see how we can go beyond the standard methods, described above, by means of time-dependent perturbation theory. This will be based upon the Covariant Evolution Operator (CEO) method mentioned above.

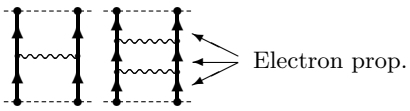

Figure 3: Graphical representation of the Green's function. The free ends are electron propagators.

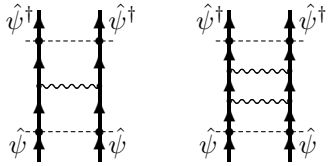

Figure 4: Graphical representation of the covariant evolution operator. The free lines are electron-field operators.

3.1 Covariant Evolution Operator (CEO)

The single-particle Green-s function can be defined (in Heisenberg representation, T is the Wick time ordering)

$$G(t,t_0) = \frac{\langle 0_{\rm H}|T[\hat{\psi}_{\rm H}(x)\hat{\psi}^\dagger_{\rm H}(x_0)]|0_{\rm H}\rangle}{\langle 0_{\rm H}|0_{\rm H}\rangle}. \tag{12}$$

The single-particle CEO can be defined analogously

$$U_{\rm Cov}(t,t_0) = \iint {\rm d}^3\boldsymbol{x}\,{\rm d}^3\boldsymbol{x}_0\,\hat{\psi}^\dagger(x)\langle 0_{\rm H}|T[\hat{\psi}_{\rm H}(x)\hat{\psi}^\dagger_{\rm H}(x_0)]|0_{\rm H}\rangle\hat{\psi}(x_0). \tag{13}$$

The Green's function is a *function*, while the CEO is an *operator* (see Figs 3 and 4).

The covariant evolution operator represents the time evolution of the *relativistic* state vector,

$$\Psi_{\rm Rel}(t) = U_{\rm Cov}(t,t_0)\,\Psi_{\rm Rel}(t_0). \tag{14}$$

This is singular due to intermediate model-space states. The *regular* part is referred to as the *Green's operator*,

$$U_{\rm Cov}(t,t_0)P = \mathcal{G}(t,t_0)\cdot PU_{\rm Cov}(0,t_0)P. \tag{15}$$

The heavy dot on the right-hand side implies that operators to the left of the dot operate on the model-space state at the position of the dot. In contrast to the definition of the Green's function (Eq. 12), the Green's-operator definition (15) is valid also in the multi-reference case.

The Green's operator acts as a *time-dependent wave operator*

$$\Psi^\alpha(t) = \mathcal{G}(t,-\infty)\Psi^\alpha_0, \tag{16}$$

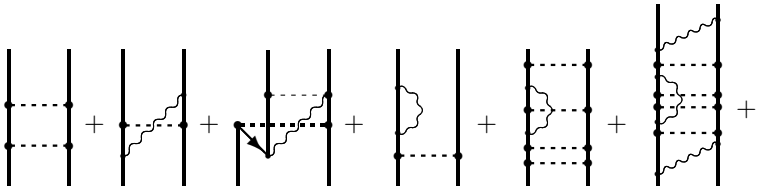

Figure 5: Iteration of the Bloch equation (17), can lead to a mixture of Coulomb and QED perturbations..

which can be compared to the wave operator of standard MBPT (3).

The Green's operator satisfies the *Bloch-type equation*

$$\boxed{\left[\mathcal{G}, H_0\right] = V\mathcal{G} - \mathcal{G}W + \left[\frac{\delta^*\mathcal{G}}{\delta\mathcal{E}}, H_0\right] W,} \tag{17}$$

where the asterisk indicates that the derivation is restricted to the last interaction. The last two terms represent model-space contributions. This equation can be compared with the standard Bloch equation (6)

$$\left[\Omega, H_0\right] = V\Omega - \Omega W. \tag{18}$$

Here, we see that the only difference lies in the extra model-space term of Eq. (17), involving the energy derivative of the interactions. This demonstrates that the perturbation expansion based upon the Green's function is completely compatible with the standard procedure.

Using the Bloch equation (17) for the Green's operator, an iterative procedure can be constructed, where time-independent as well as time-dependent interactions can be arbitrarily mixed (see Fig. 5). This implies thar also second- and higher-order QED effects can be included, provided that they are *reducible*, i.e., separable into lower-order effects. This is illustrated by the last diagram in Fig. 5. To include *irreducible* QED effects in the perturbation expansion is for the time being beyond reach. Such effects, however, can be expected to be extremely small.

4 Numerical results

The combined effect of electron correlation and first-order QED beyond second order is compared with the two-photon retardation effect (Coulomb-Breit) for the ground states of some He-like ions in Table 4. We can see that the third- and higher-order effects with first-order retardation, iare quite significant, representing 10-30% of the corresponding second-order effect. These effects are out of reach for the standard procedure presently used.

Table 4: Combination of electron correlation and first-order QED beyond second order is compared with second-order QED for the ground states of He-like ions (in eV).

Z	Two-photon	MBPT-QED beyond two-photon			
	Retarded	Retardation	Virt.Pairs	Self-energy	Vertex corr.
10	0.0033	-0.0011	0.0002		
14	0.0080	-0.0019	0.0004	0.0022	
18	0.0150	-0.0027	0.0006	0.0032	
24	0.0305	-0.0042	0.0009		
30	0.0519	-0.0057	0.0013	0.0086	
42	0.112	-0.0087	0.0019		
50		-0.011	0.002	0.017	

The calculations are performed in the Coulomb gauge in order to be able to take full advantage of the development in MBPT. The renormalization in this gauge is more complicated than in the more frequently used Feynman gauge and has never been performed before. The procedure was recently developed by Holmberg and Hedendahl [17, 18], based upon the theoretical work of Adkins [19, 20]. The values of the self-energy contributions in the table are preliminary and do not include the model-space contribution. This will be evaluated together with the vertex correction, and such calculations are presently under way.

5 Summary and conclusions

What has been presented here can be summarized in the following way:

- A procedure for time/energy-dependent perturbation theory has been developed and is now being implemented.
- Time/energy-dependent perturbations can be mixed into the many-body wave function, and the combination of electron correlation and QED can be evaluated.
- This has been applied to the ground states of He-like ions.
- This can lead to higher accuracy than the currently used methods for stationary problems, such as energy separations and atomic g-factors.
- The procedure can also be applied to dynamical processes.

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