New Approach to Many-Body-QED Calculations: Merging Quantum-Electro-Dynamics with Many-Body Perturbation

Ingvar Lindgren, Sten Salomonson, and Daniel Hedendahl

Abstract: A new method for bound-state QED calculations on many-electron systems is presented that is a combination of the non-QED many-body technique for quasi-degenerate systems and the newly developed covariant-evolution-operator technique for QED calculations. The latter technique has been successfully applied to the fine structure of excited states of medium-heavy heliumlike ions, and it is expected that the new method should be applicable also to light elements, hopefully down to neutral helium.

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1. Introduction

There exist essentially two approaches to bound-state QED calculations on many-electron systems, which we can refer to as the *low-Z* and the *high-Z approaches*, respectively.

In the low-field approach the effects of relativity and QED are expanded in powers of α and $Z\alpha$, normally starting from the Bethe-Salpeter equation [1]. This was pioneered in the 1950's by Araki [2] and Sucher [3], who evaluated all contributions to the helium energy levels to order α^3 H(artrees). Following mainly the approach of Sucher, Douglas and Kroll [4] evaluated in 1974 all contributions to the helium fine structure of order α^4 H. In the 1990's also all contributions of order α^5 H and $\alpha^5 \log \alpha$ H have been evaluated by Zhang and Drake [5, 6, 7] as well as by Pachucki and Sapirstein [8, 9, 10]. Numerical evaluation of these effects has been done particularly by Drake and coworkers [11], using accurate Hylleraas-type of wave functions. With the contributions of order α^5 H the theory has reached the level of accuracy of the experimental results for the $1s2p$ state of helium, although there are still serious discrepancies between theory and experiment.

In the high-Z approach the starting point is Dirac orbitals and electron propagators (Green's functions), generated in the field of the nucleus, which in terms of free electrons correspond to expansions with nuclear interactions, as illustrated in Fig. 1. With these orbitals/propagators the covariant multi-(one-, two-,...) photon exchange, illustrated in Fig. 2, is evaluated numerically. This has been the approach of various groups and successfully applied to highly charged ions (see Refs [12, 13, 14], for further references).

For an isoelectronic sequence, as the heliumlike systems, the effect of multi-photon exchange decreases roughly by a factor of Z for each additional photon. This implies that the high-Z approach converges rapidly for heavy elements but quite slowly for light elements. For practical reasons, it is at present not feasible to evaluate the exchange of more than two covariant photons in this way, which,

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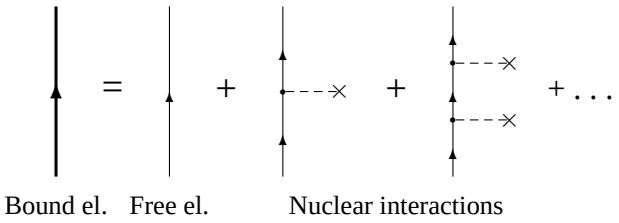

Fig. 1. The bound electron orbital, generated in the field of the atomic nucleus, can be represented by a free electron with nuclear potential interactions, each corresponding to a factor of $Z\alpha$ in the analytical expansion.

however, leads to good accuracy for highly charged ions. For light elements, on the other hand, where the electron correlation is relatively strong, this approach is not feasible.

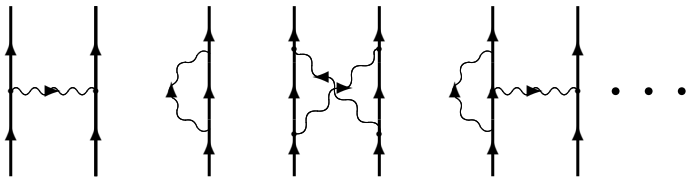

Fig. 2. Examples of covariant multi-photon exchange diagrams.

There is presently a great interest in the fine structure of the lowest ^3P state of neutral helium, both experimentally and theoretically, since a comparison between theory and experiment can yield an accurate value of the fine-structure constant α. Very accurate measurement of the separation $^3P_1 - ^3P_0$ has been performed [15] and even more accurate experiments are under way as reported at the ICAP 2004 conference in Rio de Janeiro. Accurate QED calculations can only be performed with the low-Z approach, but there is some confusion about the theoretical results [10, 16, 11, 17]. The results disagree, and the most complete calculation of Drake [11] differs by 4-5 standard deviations from experiments for the $^3P_1 - ^3P_0$ transition (using the accepted value of α) and even more for the $^3P_2 - ^3P_1$ transition. The reason for this problem is not clear. It is obvious that the analytic approach becomes drastically more complicated — and more error prone — for each order of perturbation, and it is questionable if it will ever be possible to go beyond the order presently reached.

In the present paper we shall discuss an alternative approach that may make it possible to extend the numerical approach to low Z, possibly as far as down to neutral helium. This is based upon the *covariant-evolution-operator approach*, which we have successfully used in evaluating the fine-structure separations of heliumlike ions down to $Z = 9$ [18, 14]. In the proposed extension we shall base the evaluation on correlated pair functions, instead of hydrogenic Dirac orbitals, in this way including the dominating effect of electron correlation into the QED calculations.

In principle, we will be able to evaluate all effects due to so-called Coulomb-ladder diagrams as well as those involving a single transverse photon with arbitrary number of Coulomb crossings. This will constitute a possibility to test the analytical approach.

The contributions due to two transverse photons are of two kinds, in the papers quoted above denoted by $\Delta E^{T\cdot T}$ and $\Delta E^{T\times T}$, representing reducible and irreducible effects, respectively. It has been shown by Zhang [6] that the exchange of three transverse photons does not affect the fine structure

to order α^5 H. We will be able to evaluate the reducible two-photon effect by iterating single-photon exchange, and therefore the only effect that we will not be able to treat numerical on this level in the near future is the irreducible two-photon effect. That has then to be included by means of an analytical approximation. In addition, of course, our approach will automatically include many effects of higher orders, but not in a complete manner.

To what extent we will be able to evaluate the radiative effects numerically is presently under investigation. To begin with, we shall use the phenomenological approach, using the anomalous magnetic moment of the electron, which will be correct to order α^4.

As a background to the description of our new technique, we shall first briefly summarize the non-QED many-body technique for quasi-degenerate systems, followed by a summary of the high-Z approaches, the S-matrix method and the recently introduced covariant-evolution-operator method [18, 14].

2. Many-Body Theory

In the standard many-body perturbation theory (MBPT) we want to solve the Schrödinger equation for a number of target states

$$H\,\Psi^\alpha = E^\alpha\,\Psi^\alpha \qquad (\alpha = 1, 2\cdots d) \tag{1}$$

The Hamiltonian is partitioned into an unperturbed model Hamiltonian and a perturbation

$$H = H_0 + H' \tag{2}$$

For each target state we have a model state, $\Psi_0^a = P\Psi^a$, which is an eigenfunction of H_0 and confined to a model space with the projection operator P.

The *wave operator* transforms the model states to the target states $\Psi^\alpha = \Omega\,\Psi_0^\alpha$ $(\alpha = 1, 2\cdots d)$ and satisfies the generalized Bloch equation [19]

$$\big[\Omega, H_0\big]P = \big(H'\,\Omega - \Omega\,PH'\Omega\big)P \tag{3}$$

assuming intermediate normalization $P\Omega P = P$.

Projecting the Schrödinger equation (1) on the model space yields

$$PH\Omega\,\Psi_0^\alpha = E^\alpha\,\Psi_0^\alpha \tag{4}$$

which shows that the model functions are eigenfunctions of the *effective Hamiltonian* $H_{\rm eff} = PH\Omega P$ with the eigenvalues equal to the exact eigenvalues of the target states.

Using second quantization, the wave operator can be separated into one-, two-,..body parts [19]

$$\Omega = 1 + \Omega_1 + \Omega_2 + \cdots \tag{5}$$

and insertion into the Bloch equation (3) leads to the equations

$$\big[\Omega_n, H_0\big]P = \big(H'\,\Omega - \Omega\,PH'\Omega\big)_n P \tag{6}$$

If we consider heliumlike systems, starting with hydrogenic orbitals generated in the field of the nucleus, the wave operator has only a two-body component, $\Omega = 1 + \Omega_2$, satisfying the *pair equation*

$$\big[\Omega_2, H_0\big]P = \big(H' + H'\Omega_2\big)_2 P - \Omega_2 H'_{\rm eff,2} \tag{7}$$

where H' is the Coulomb interaction $1/r_{12}$ and $H'_{\rm eff} = PH'\Omega P$ is the perturbative part of the effective Hamiltonian (4), $H_{\rm eff} = PH_0P + H'_{\rm eff}$. The last term in the pair equation (7) represents so-called folded diagrams. This yields the matrix elements of the wave operator

$$\langle rs|\Omega_2|ab\rangle = \frac{\langle rs|1/r_{12}|ab\rangle + \langle rs|1/r_{12}|tu\rangle\langle tu|\Omega_2|ab\rangle}{\varepsilon_a + \varepsilon_b - \varepsilon_r - \varepsilon_s + \Delta} \tag{8}$$

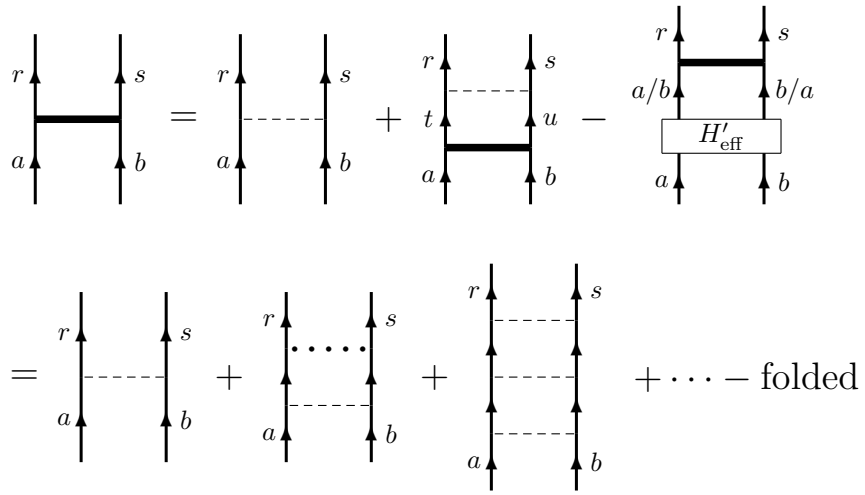

Fig. 3. The pair function for a two-electron system is equivalent to an infinite sequence of ladder diagrams (including the folded diagrams).

summed over the intermediate states $|tu\rangle$, where $\Delta = \langle ab|H'_{\rm eff,2}|ab\rangle$ (incl. exchange) is due to the folded diagrams. The state $|ab\rangle$ lies in the model space and the states $|rs\rangle$ and $|tu\rangle$ outside this space (ε_a etc. are the orbital energy eigenvalues).

The pair equation (7) can be solved non-perturbatively by recursion, which corresponds to a perturbative expansion to all orders and represents the exact solution of the Schrödinger equation for this system. This can be represented graphically as in Fig. 3. For the numerical solution we use the method of discretization, developed by Salomonson and Öster [20, 21].

The pair functions are used to evaluate the elements of the effective Hamiltonian (4) — diagonal as well as non-diagonal — and the diagonalization then yields the model functions and the energies with corresponding accuracy. This approach is particularly effective in the case of *quasi-degeneracy*, where unperturbed states can be strongly mixed. By including such states in the model space, their mixing will be accounted for to all orders of perturbation theory.

A good illustration of the power of the method is the application to the fine structure of the $1s2p\,^3P$ state of heliumlike ions, where it has been shown to converge in all cases down to neutral helium [22]. The conventional approach with a single model function, on the other hand, fails for light elements, and even model functions that are eigenfunctions of the first-order effective Hamiltonian does not lead to convergence for $Z \leq 6$ [23].

3. S-matrix formulation

The standard approach for bound-state QED calculations is the S-matrix formulation [12]. This is based upon the *time-evolution operator*, defined by $\Psi(t) = U(t,t_0)\,\Psi(t_0)$. This can be expanded as

$$U(t,t_0) = 1 + \sum_{n=1}^{\infty} \frac{(-\mathrm{i})^n}{n!} \int_{t_0}^{t} \mathrm{d}^4x_n \ldots \int_{t_0}^{t} \mathrm{d}^4x_1\, T_{\rm D}\big[\mathcal{H}'_{\rm I}(x_n)\ldots\mathcal{H}'_{\rm I}(x_1)\big] \tag{9}$$

where $T_{\rm D}$ is the Wick time-ordering operator and

$$\mathcal{H}'_{\rm I}(x) = -e\psi^\dagger(x)\,\alpha^\mu A_\mu(x)\psi(x) \tag{10}$$

is the perturbation in the form of the electron-field interaction in the interaction picture [24]. e is here the absolute value of the electronic charge (positive number), $\psi(x)/\psi^\dagger(x)$ represent the electron-field operators and $A_\mu(x)$ the electromagnetic field.

A damping factor $\mathcal{H}'_{\rm I}(x) \rightarrow \mathcal{H}'_{\rm I}(x)\,e^{-\gamma|t|}$ is introduced, so that the Hamiltonian approaches the unperturbed Hamiltonian, when $t_0 \rightarrow \pm\infty$. The evolution operator from the unperturbed state for the exchange of a single photon between two electrons is given by (using relativistic units, $m = c = \hbar = \epsilon_0 = 1$)

$$\begin{aligned} SU^{(2)}(t',-\infty) &= -\frac{e^2}{2}\iint_{-\infty}^{t'} \mathrm{d}^4x_1\,\mathrm{d}^4x_2\,\psi^\dagger(x'_1)\psi^\dagger(x'_2) \\ &\times \alpha_1^\mu\,\mathrm{i}D_{\mathrm{F}\mu\nu}(x_1-x_2)\,\alpha_2^\nu\,\psi(x_1)\,\psi(x_2)\,\mathrm{e}^{-\gamma(|t_1|+|t_2|)} \end{aligned} \tag{11}$$

and illustrated in Fig. 4. $D_{\mathrm{F}\mu\nu}(x_1-x_2)$ is here the photon propagator, represented by the contraction of the electromagnetic-field operators of the perturbations $\mathcal{H}'_{\rm I}(x_1)$ and $\mathcal{H}'_{\rm I}(x_2)$. The S matrix is defined by $S = U(\infty,-\infty)$. Performing the time integrations yields for the single-photon exchange

$$\langle rs|S^{(2)}|ab\rangle = -2\pi\mathrm{i}\,\delta(\varepsilon_a+\varepsilon_b-\varepsilon_r-\varepsilon_s)\,\langle rs|V_{\rm eq}|ab\rangle \tag{12}$$

and the corresponding energy shift

$$\Delta E = \langle rs|H^{(1)}_{\rm eff}|ab\rangle = \delta(\varepsilon_a+\varepsilon_b-\varepsilon_r-\varepsilon_s)\,\langle rs|V_{\rm eq}|ab\rangle \tag{13}$$

Here, $V_{\rm eq} = \alpha_1^\mu\,\mathrm{i}D_{\mathrm{F}\mu\nu}(x_1-x_2)\,\alpha_2^\nu$ is the *effective interaction* and in the Feynman gauge given by

$$V_{\rm eq}(q) = \int_0^\infty \mathrm{d}k\,f(k)\,\frac{2k}{q^2-k^2+\mathrm{i}\eta} \tag{14}$$

where

$$f(k) = -\frac{e^2}{4\pi^2\,r_{12}}\,(1-\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2)\,\sin(kr_{12})$$

and $q = \varepsilon_a-\varepsilon_r = \varepsilon_s-\varepsilon_b$.

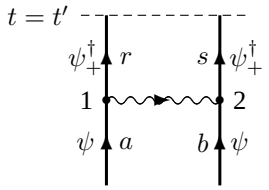

Fig. 4. Graphical representation of the standard evolution operator for single-photon exchange. The outgoing lines represent here positive-energy electron states.

The delta factor above shows that energy must be conserved in the S matrix. Therefore, off-diagonal elements of the effective Hamiltonian between states with different unperturbed energies cannot be evaluated, which is a serious limitation, implying that the method cannot be applied to the case of quasi-degeneracy, as described in the MBPT section. An additional shortcoming is that no information of the wave function is obtained.

4. Covariant evolution-operator method

In order to remedy the shortcomings of the S-matrix method for bound-state calculations, we have introduced a modification, referred to as the *covariant evolution-operator method* [18, 14]. We then return to the evolution operator (11), and in order to make this covariant we allow the outgoing orbitals to represent positive- as well as negative-energy states. This leads to the expression

$$U^{(2)}_{\rm Cov}(t',-\infty) = -\frac{e^2}{2}\iint {\rm d}^3\boldsymbol{x}'_1 {\rm d}^3\boldsymbol{x}'_2\, \psi^\dagger(x'_1)\psi^\dagger(x'_2)$$
$$\times \iint_{-\infty}^{\infty} {\rm d}^4x_1\, {\rm d}^4x_2 {\rm i}S_{\rm F}(x'_1,x_1)\, {\rm i}S_{\rm F}(x'_2,x_2)\, \alpha_1^\mu\, {\rm i}D_{{\rm F}\mu\nu}(x_2-x_1)\, \alpha_2^\nu\, \psi(x_2)\, \psi(x_1)\, {\rm e}^{-\gamma(|t_1|+|t_2|)} \qquad (15)$$

illustrated by the time-ordered diagrams in Fig. 5. $S_{\rm F}(x',x)$ is the *electron propagator* or *single-electron Green's function*, represented by the internal lines of the right-most diagram.

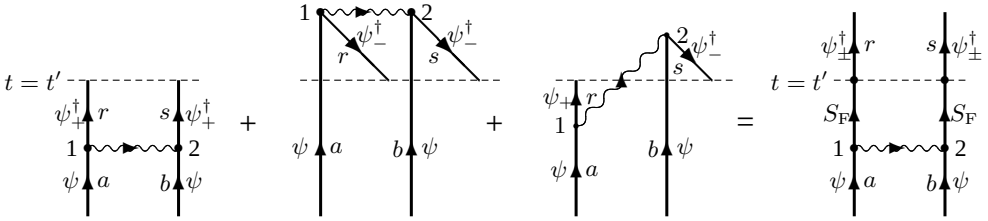

Fig. 5. Graphical representation of the covariant evolution operator for single-photon exchange. The outgoing lines can here represent positive- as well as negative-energy states.

Evaluating the single-photon exchange (15) yields the first-order effective Hamiltonian

$$H^{(1)}_{\rm eff} = V_{\rm eq}(q,q') = \int_0^\infty {\rm d}k\, f(k) \left[\frac{1}{q \mp (k - {\rm i}\gamma)} + \frac{1}{q' \mp (k - {\rm i}\gamma)}\right] \qquad (16)$$

where $q = \varepsilon_a - \varepsilon_r,\ q' = \varepsilon_b - \varepsilon_s$ and $\mp$ represents hole/particle states. In contrast to the corresponding S-matrix expression (12), energy need not here be conserved. This means that also non-diagonal elements can be evaluated, which is needed in order to apply the method to quasi-degeneracy as described above. The covariant evolution operator also yields information about the wave function. The matrix element of the first-order wave operator is given by

$$\langle rs|\Omega|ab\rangle = \frac{\langle rs|V_{\rm eq}(q,q')|ab\rangle}{q+q'} \qquad (17)$$

We have applied the covariant-evolution-operator method to evaluate the fine structure of the $1s2s^3P$ state of some heliumlike ions [18, 14], and the results are exhibited in Table 1, where comparison is made with the experimental results as well as with calculations of Drake [25, 11] and Plante et al. [23] (We refer to Refs [18, 14] for more detailed references and discussions). Our calculation represents the first numerical evaluation of QED effects of the fine structure of heliumlike ions, including the strongly mixed $^3P_1$ state. Previous calculations, using the S-matrix method, has been restricted to the pure states $^3P_2$ and $^3P_0$ [26].

An alternative approach for QED calculations on quasi-degenerate states is the *two-times Green's-function method*, developed by Shabaev and coworkers [13]. At least in its present form, this method does not yield any information about the wave function (wave operator) and can therefore not be used as a basis for the combined QED-MBPT approach to be presented in the next section.

Table 1. The $1s2p\,^3P$ fine structure of He-like ions. Values for Z=2,3 given in MHz and the remaining in μHartree.

Z	$^3P_1 - ^3P_0$	$^3P_2 - ^3P_0$	$^3P_2 - ^3P_1$	
2	29616.9509(9)		2291.1759(10)	Expt'l
	29616.94642(18)		2291.15462(31)	Drake
3	155704.27(66)		-62678.41(66)	Expt'l
	155703.4(1,5)		-62679.4(5)	Drake
9	701(10)		4364,517(6)	Expt'l
	680	5050	4362(5)	Drake
	690	5050	4364	Plante
	690	5050	4364	Present work
10	1371(7)	8458(2)		Expt'l
	1361(6)	8455(6)	265880	Drake
	1370	8469	265860	Plante
	1370	8460	265880	Present work
18		124960(30)		Expt'l
		124810(60)		Drake
		124942		Plante
		124940		Present work

5. Combined high- and low-Z approach

In this section we shall describe the new approach to many-body-QED calculations that is under development at our laboratory. This is a combination of the many-body approach for quasi-degeneracy, described in section 2, and the covariant-evolution-operator method for bound-state QED, described in the previous section.

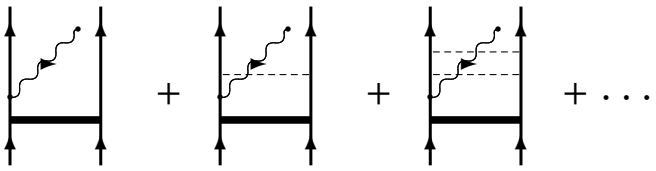

Fig. 6. Graphical representation of a pair function (Fig. 3) with uncontracted photon (folded diagrams left out).

The basic idea is to start with the pair functions, illustrated in Fig. 3, and to add the perturbation (10), representing the interaction between the electromagnetic field and *one* of the electrons. This is illustrated by the leftmost diagram in Fig. 6. Further iterations of the pair equation yields additional Coulomb interactions, as represented by the remaining diagrams of the figure. (In principle, these interactions can also be instantaneous Breit interactions.) This requires one pair function for each momentum k of the photon.

The photon can be closed by contracting with another perturbation (10), either on the other electron, which yields covariant photon interaction between the electrons or on the same electron, which yields a self-energy interaction (the latter with the proper renormalization). This yields diagrams of the type illustrated in Fig. 7.

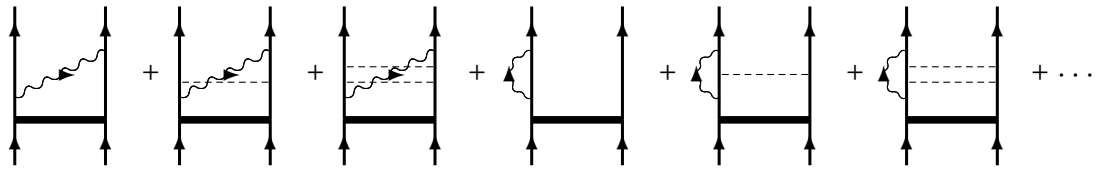

Fig. 7. The uncontracted photon in Fig. 6 can be closed by interacting with the same or the other electron.

Finally, the pair function can be iterated further with Coulomb interactions, which yields diagrams of the type illustrated in Fig. 8. The first diagram represents a complete covariant photon between the electrons, evaluated with relativistic correlated wave function. The next diagram represents the dominating part of the crossed-photon diagram, where one of the photons is retarded and the other is instantaneous (Coulomb or Coulomb-Breit) and so on. The situation is analogous for the self-energy diagrams, where the additional interactions yield vertex corrections. For the time being it does not seem feasible to treat more than one covariant photon in this manner.

It has been shown by Zhang and Drake [6, 27] that one and two transverse photons with arbitrary number of Coulomb crossings affect the helium fine structure to order α^5 H, while the exchange of three transverse photons does not enter on this level.

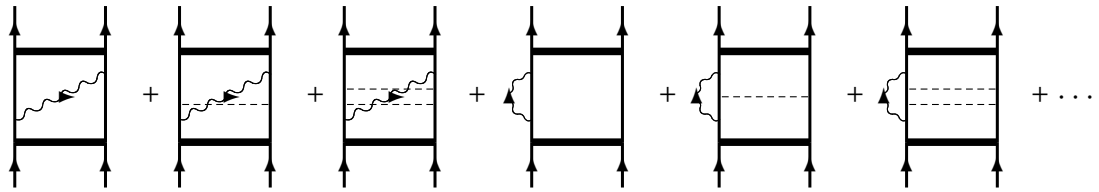

Fig. 8. Further iterations of the pair functions in Fig. 7 yields QED effects evaluated with fully correlated relativistic wave functions.

6. Summary and discussion

Here we have outlined a method for many-body-QED calculations that is presently under development. It is basically a combination of the many-body technique for quasi-degeneracy and the recently developed covariant-evolution-operator technique for bound-state calculations. We expect the method to be applicable to all nuclear charges, but our main interest will be on light elements, where the traditional high-Z approaches fail.

The use of relativistic bound-state orbitals/propagators implies that our numerical results will automatically correspond to many terms in the expansion in powers of $Z\alpha$ of the analytical low-Z approach. In addition we can evaluate the effect of a single transverse photon with arbitrary Coulomb crossings, as illustrated in Fig. 8. The only non-radiative effect entering in order α^5 H that we cannot evaluate numerically at present is the irreducible two-photon effect, which then has to be included analytically. To begin with, the radiative effects will be included using analytical expressions.

Our goal is to be able to evaluate the fine-structure separation of neutral helium accurately, and believe that a combination of the numerical and analytical approaches will have the best probability for success. It is still an open question, though, what accuracy can actually be reached.

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