A Numerical Procedure for Combined Many-Body-QED Calculations

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A procedure for relativistically covariant many-body perturbation theory (MBPT) has been developed, and some numerical implementation has been started. The procedure is based upon the previously introduced covariant evolution operator, which is a field-theoretical concept, closely related to MBPT. The procedure leads to all kinds of relativistic and quantum-electrodynamical (QED) effects, and can be shown for two-particle systems to lead to the Bethe-Salpeter equation. In the implementation an extension to the photonic Fock space is made, where the number of photons no longer is constant.

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I. INTRODUCTION

The non-relativistic Many-Body Perturbation Theory (MBPT) for atomic and molecular systems is very well developed, and a number of effective techniques have been appeared. In this group of methods we also include so-called "all-order" techniques, like the "Exponential Ansatz" or Coupled-Cluster Approach (CCA) [1]. Here, the electron correlation can be treated essentially to arbitrary order. All these methods have the important property of being *size extensive*, which means that the energy scales linearly with the size of the system. In addition, these methods can also treat the *quasi-degeneracy* problem with closely spaced energy levels by means of an effective-Hamiltonian approach. It is well-known that such an approach in many cases can lead to convergence problems, due to "intruder states". Nowadays, there exist several effective ways of circumventing these problems by using an incomplete model space [2, 3] or an "intermediate effective Hamiltonian" [4]. We shall not be particularly concerned with this problem here, but the reader is referred to other contributions to this volume, particularly devoted to the problem. Here, we shall be particularly concerned with the relativity problem and how the MBPT/CCA procedures can be extended to the relativistic regime in a fully covariant way.

The standard procedure for relativistic MBPT is to use the projected *Dirac-Coulomb-Breit* (DCB) Hamiltonian, introduced by Sucher in 1980 [5], also known as the *no-virtual-pair approximation* (NVPA), (in relativistic units: $m = c = \hbar = \epsilon_0 = 1$)

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

Here, h_D is the single-electron Dirac Hamiltonian and

$$H_B = -\frac{e^2}{8\pi} \sum_{i<j} \Big[\frac{\boldsymbol{\alpha}_i \cdot \boldsymbol{\alpha}_j}{\boldsymbol{r}_{ij}} + \frac{(\boldsymbol{\alpha}_i \cdot \boldsymbol{r}_{ij})(\boldsymbol{\alpha}_j \cdot \boldsymbol{r}_{ij})}{r_{ij}^3} \Big] \tag{2}$$

is the instantaneous Breit interaction. Λ_+ is an operator projecting out the single-electron states of positive energy, thereby avoiding the well-known Brown-Ravenhall disease [6].

The DCB Hamiltonian (1) is NOT relativistically covariant, but it is correct to order α^2 Hartrees. In order to go beyond that level, a different approach is required. Conventionally, we shall refer to all effects beyond the NVPA, i.e., of order α^3 and beyond, as QED effects. These are of two kinds, *non-radiative effects*, due to retardation and to virtual electron-positron pairs, and *radiative effects*, including electron self energy, vacuum polarization and vertex corrections, illustrated in Fig. 1.

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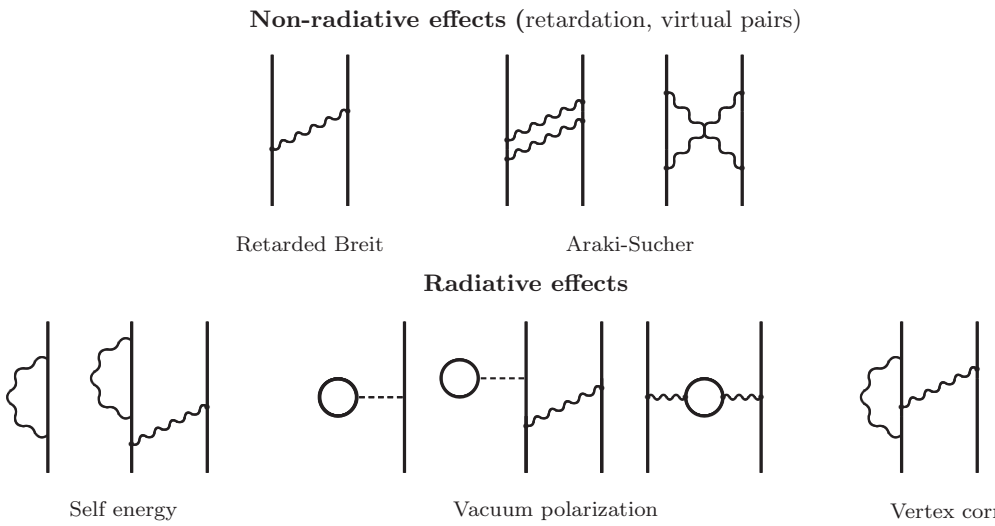


FIG. 1: Graphical representation the lowest-order QED effects. These are of order α^3 Hartrees and beyond.

The first fully relativistically covariant treatment of a bound-state problem is represented by the *Bethe-Salpeter equation* (BSE), first derived for two-particle systems in 1951 by Salpeter and Bethe [7] and by Gell-Mann and Low [8]. This can be expressed as an implicit equation for the wave function

$$\Psi(E) = G_0(E)\,\Sigma(E)\,\Psi(E) \tag{3}$$

where $G_0(E)$ is the zeroth-order two-particle Green's function, $\Sigma(E)$ is the two-particle self-energy operator, and E is the energy of the system. The Green's function and the self energy are here *four-time operators*, with individual initial and final times for the two particles [26]. In most applications the original BSE is replaced by an effective-potential approximation [9]

$$(E - H_0)\Psi(E) = \mathcal{V}(E)\Psi(E) \tag{4}$$

where the potential $\mathcal{V}$ is given by all *irreducible* multi-photon exchange between the electrons (see Fig. 2). A diagram is said to be reducible if it can be separated into two diagrams by a horizontal cut that does not cross any photon line. The remaining diagrams are irreducible. The potential is identical to the self-energy of the BSE (3), apart from the fact that the initial and final times for the two particles are assumed to be the same. For atomic and molecular problems the error in this approximation—if any—is negligible.

The BSE (4) is normally solved perturbatively by means of the Brillouin-Wigner perturbation expansion. In atomic physics this was first applied by Sucher [10, 11], and later by Douglas and Kroll [12] and by Drake and associates [13, 14]. Our goal, however, is to obtain a perturbative expansion based upon the *Rayleigh-Schrödinger perturbation expansion*, which would be compatible with the well-developed non-relativistic techniques, such as the linked-diagram and the coupled-cluster approaches.

II. FIELD-THEORETICAL APPROACH

In order to develop a relativistically covariant many-body perturbation expansion, we have to rely on field theory, and, therefore, we turn to time-dependent perturbation theory. We then partition the Hamiltonian into a time-independent model Hamiltonian and a time-dependent perturbation

$$H = H_0 + H(t) \tag{5}$$

The *time-evolution operator*, which represents the evolution of the state vector in the interaction picture (IP) with time, is defined

$$|\Psi_{\rm I}(t)\rangle = U(t,t_0)\,|\Psi_{\rm I}(t_0)\rangle \tag{6}$$

This satisfies the equation

$$\mathrm{i}\frac{\partial}{\partial t}\,U(t,t_0) = H'_{\rm I}(t)\,U(t,t_0) \tag{7}$$

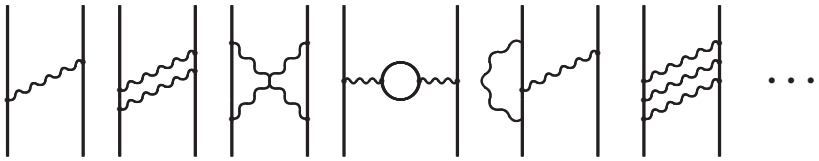


FIG. 2: The effective-potential of the Bethe-Salpeter equation (4) is represented by all *irreducible* multi-photon exchange diagrams between the electrons.

where $H'_{\rm I}(t)$ is the (time-dependent) perturbation in IP, with the solution [15]

$$U(t,t_0) = 1 + \sum_{n=1}^{\infty} \frac{(-{\rm i})^n}{n!} \int_{t_0}^{t} {\rm d}^4x_n \cdots \int_{t_0}^{t} {\rm d}^4x_1 \; T_{\rm D}\big[\mathcal{H}'_{\rm I}(x_n)\mathcal{H}'_{\rm I}(x_{n-1}) \cdots \mathcal{H}'_{\rm I}(x_1)\big]. \tag{8}$$

$T_{\rm D}$ is a time-ordering operator, and $\mathcal{H}'_{\rm I}(x)$ is the perturbation *density*, defined by

$$H'_{\rm I}(t) = \int {\rm d}^3\boldsymbol{x}\, \mathcal{H}'_{\rm I}(t,\boldsymbol{x}). \tag{9}$$

Here, we assume that the perturbation density is given by the interaction between electrons and the quantized electro-magnetic field [16]

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

where $\hat{\psi}_{\rm I}$, $\hat{\psi}^\dagger_{\rm I}$ are the electron field operators, α^μ the Dirac alpha operators and A_μ is the radiation field.

III. COVARIANT EVOLUTION-OPERATOR APPROACH. GREEN'S OPERATOR

A. The covariant evolution operator

In field theory the interaction between the electrons is represented by the exchange of virtual photons. The exchange of a single photon is represented by the contraction of *two* perturbations (10), which leads to the evolution operator (8)

$$U^{(2)}(t',t_0) = -\frac{1}{2}\iint_{t_0}^{t'} {\rm d}^4x_1{\rm d}^4x_2\, \hat{\psi}^\dagger_{\rm I+}(x_1)\hat{\psi}^\dagger_{\rm I+}(x_2)\, {\rm i}I(x_1,x_2)\, \hat{\psi}_{\rm I+}(x_2)\hat{\psi}_{\rm I+}(x_1)\, {\rm e}^{-\gamma(|t_1|+|t_2|)} \tag{11}$$

Here, $I(x_1,x_2)$ represents the contraction of two radiation-field operators, which is essentially the Feynman photon propagator. γ is the adiabatic damping factor, which eventually goes to zero. The integrations are over all space coordinates and time coordinates as indicated. $\hat{\psi}_{\rm I+}$, $\hat{\psi}^\dagger_{\rm I+}$ are the positive-energy part of the electron-field operators. This operator is *non-covariant*, since time evolves only in the positive direction and only positive-energy states are involved. It can, however, be made *covariant* by inserting zeroth-order Green's functions (electron propagators) on the in- and outgoing lines [17, 18]

$$\begin{aligned} U^{(2)}_{\rm Cov}(t',t_0) \;=\; & -\frac{1}{2}\iint {\rm d}^3\boldsymbol{x}'_1{\rm d}^3\boldsymbol{x}'_2\, \hat{\psi}^\dagger_{\rm I}(x'_1)\hat{\psi}^\dagger_{\rm I}(x'_2) \iint {\rm d}^4x_1{\rm d}^4x_2\, G_0(x'_1,x'_2;x_1,x_2) \\ & \times \iint {\rm d}^3\boldsymbol{x}_{10}{\rm d}^3\boldsymbol{x}_{20}\, {\rm i}I(x_1,x_2)\, G_0(x_1,x_2;x_{10},x_{20})\, \hat{\psi}_{\rm I}(x_{20})\hat{\psi}_{\rm I}(x_{10}) \end{aligned} \tag{12}$$

Here, the times t_1 and t_2 of the interaction run over *all times*, and positive- as well as negative-energy states are involved. The standard and covariant evolution operators for single-photon exchange are represented graphically in Fig. 3.

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

$$|\Psi_{\rm I,Rel}(t)\rangle = U_{\rm Cov}(t,t_0)|\Psi_{\rm I,Rel}(t_0)\rangle \tag{13}$$

in analogy with the standard evolution operator (6).

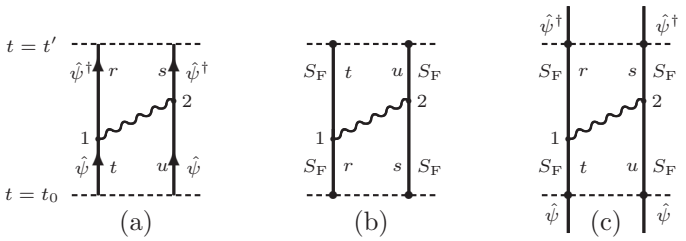


FIG. 3: Graphical representation of the standard covariant-evolution operator (a), Green's operator (b) and the covariant-evolution operator/Green's function (c) for single-photon exchange.

B. The reduced covariant evolution operator or Green's operator

The covariant evolution operator is generally singular and can be separated into regular and singular parts. The former is referred to as the *reduced covariant evolution operator* ($\widetilde{U}$) and defined by [18]

$$U(t)P = P + \widetilde{U}(t)P \cdot PU(0)P \tag{14}$$

Due to its close analogy with the Green's function, we introduce the term *Green's operator* for this part and denote it by $\mathcal{G}(t) \equiv \widetilde{U}$. The definition above leads to the expansion

$$\mathcal{G}(t)P = U(t)P - P - \mathcal{G}(t)P \cdot P\mathcal{G}(0)P - \mathcal{G}(t)P \cdot P\mathcal{G}(0)P \cdot P\mathcal{G}(0)P - \cdots \tag{15}$$

The heavy dot indicates that the part to the left evolves from the intermediate model-space state. The negative terms are referred to as "counter-terms" and have the effect of eliminating (quasi-)singularities of the evolution operator. This leads to some finite residuals that are analogous to the "folded" terms of standard MBPT [1].

The close analogy between the Green's operator and the Green's function is illustrated for single-photon exchange in Fig. 3. This analogy verifies that the covariant evolution operator and the Green's operator are field-theoretical concepts.

C. Single-photon exchange

The covariant evolution operator/Green's operator for single-photon exchange is given by [18]

$$\langle rs|\mathcal{G}(t)|ab\rangle = \big\langle rs\big|\mathrm{e}^{-\mathrm{i}t(E_0-\varepsilon_r-\varepsilon_s)}\Gamma_Q V(E_0)\big|ab\big\rangle \tag{16}$$

where $E_0 = \varepsilon_a + \varepsilon_b$ is the initial energy and Γ_Q is the *resolvent*

$$\Gamma_Q = \frac{Q}{E_0 - H_0} \tag{17}$$

In the Coulomb gauge, which is natural to use in many-body calculations, the potential can be separated into an *instantaneous* and a *retarded* part,

$$V(\mathcal{E}) = V_\mathrm{I} + V_\mathrm{Ret}(\mathcal{E}), \tag{18}$$

where only the latter is energy dependent. The instantaneous part is the Coulomb interaction

$$V_\mathrm{I} = \frac{e^2}{4\pi r_{12}}, \tag{19}$$

and the retarded part is given

$$\langle rs|V_\mathrm{Ret}(\mathcal{E})|tu\rangle = \Big\langle rs\Big|\int \mathrm{d}k\, f(\boldsymbol{x}_1, \boldsymbol{x}_2, k)\Big[\frac{1}{\mathcal{E} - \varepsilon_r - \varepsilon_u - (k - \mathrm{i}\eta)_r} + \frac{1}{\mathcal{E} - \varepsilon_s - \varepsilon_t - (k - \mathrm{i}\eta)_s}\Big]\Big|tu\Big\rangle \tag{20}$$

considering both time orderings. The subscript r represents the sign of ε_r. The function $f(\boldsymbol{x}_1, \boldsymbol{x}_2, k)$ is in Coulomb gauge given by

$$f_C(k) = \frac{e^2}{4\pi^2}\left[-\boldsymbol{\alpha_1}\cdot\boldsymbol{\alpha_2}\,\frac{\sin(kr_{12})}{r_{12}} + (\boldsymbol{\alpha_1}\cdot\boldsymbol{\nabla_1})\,(\boldsymbol{\alpha_2}\cdot\boldsymbol{\nabla_2})\,\frac{\sin(kr_{12})}{k^2\, r_{12}}\right] \tag{21}$$

with k being the photon momentum. The first term represents the *Gaunt* part and the second term the *scalar-retardation* part, together forming the *Breit interaction* (which also has an instantaneous part).

D. Connection to MBPT

We have seen that the Green's operator is a field-theoretical concept. At the same time this operator is closely related to the operators of standard MBPT [18]. The open part (operating from the model space to the complementary space) yields a covariant form of the MBPT wave operator

$$\boxed{\Omega^{\rm Cov} = 1 + \mathcal{G}_{\rm op}(0)} \tag{22}$$

and the closed part (operating within the model space) yields the covariant form of the effective Hamiltonian, $H_{\rm eff}^{\rm Cov} = PH_0P + V_{\rm eff}^{\rm Cov}$,

$$\boxed{V_{\rm eff}^{\rm Cov} = P\Big[{\rm i}\frac{\partial}{\partial t}\mathcal{G}(t)\Big]_{t=0}P} \tag{23}$$

In order to illustrate these rules, we consider the single-photon exchange above. From the rule (22) the expression (16) leads to

$$\langle rs|\Omega^{\rm Cov}|ab\rangle = \frac{\big\langle rs\big|V(E_0)\big|ab\big\rangle}{E_0 - \varepsilon_r - \varepsilon_s} \tag{24}$$

and the rule (23) to

$$\langle rs|V_{\rm eff}^{\rm Cov}|ab\rangle = \big\langle rs|V(E_0)\big|ab\big\rangle \tag{25}$$

If V is energy independent, these results agree with those of time-independent many-body perturbation theory. This analogy holds in all orders.

IV. PERTURBATION EXPANSION

From the definition of the Green's operator (14) and the relation (24) the first-order wave operator is given by

$$\Omega^{\rm Cov(1)} = \mathcal{G}_{\rm op}^{(1)}(0) = \Gamma_Q V(E_0) \tag{26}$$

where Γ_Q is the resolvent (17). In second order the evolution operator becomes, after eliminating singularities by means of the counter terms (15),

$$\Omega^{\rm Cov(2)} = \Gamma_Q V(E_0)\,\Omega^{\rm Cov(1)} + \Big(\frac{\delta\Omega^{\rm Cov(1)}}{\delta\mathcal{E}}\Big)_{E_0} V_{\rm eff}^{\rm Cov(1)}(E_0) \tag{27}$$

where $V_{\rm eff}^{\rm Cov(1)} = PV\Omega^{\rm Cov(1)}P$. Performing the differentiation of the first-order wave operator, leads to

$$\Omega^{\rm Cov(2)} = \Gamma_Q V\,\Omega^{\rm Cov(1)} - \Gamma_Q\,\Omega^{\rm Cov(1)}V_{\rm eff}^{\rm Cov(1)}(E_0) + \Gamma_Q\Big(\frac{\partial V(\mathcal{E})}{\partial\mathcal{E}}\Big)_{E_0} V_{\rm eff}^{\rm Cov(1)}(E_0) \tag{28}$$

Here, the first two terms correspond exactly to those of the standard Bloch equation, the second one being the so-called "folded" term. The last term is caused by the energy dependence of the potential.

When this procedure is carried out to all orders, it can be shown that it leads to [19]

$$\Omega^{\rm Cov} = \Gamma_Q\mathcal{V}(E)\,\Omega^{\rm Cov} - \Gamma_Q\,\Omega^{\rm Cov}\,\mathcal{V}_{\rm eff}^{\rm Cov}(E) \tag{29}$$

or

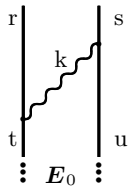
$$(E_0 - H_0)\,\Omega^{\rm Cov} = \mathcal{V}(E)\,\Omega^{\rm Cov} - \Omega^{\rm Cov}\mathcal{V}_{\rm eff}^{\rm Cov}(E) \tag{30}$$

where we have now replaced the single-photon potential by the complete multi-photon potential $\mathcal{V}$ in Fig. 2 and $V_{\rm eff}^{\rm Cov}$ by $\mathcal{V}_{\rm eff}^{\rm Cov} = P\mathcal{V}\Omega^{\rm Cov}P$. This is exactly the Bethe-Salpeter equation in the effective-potential form (4), which *verifies the relativistic covariance of the procedure applied.*

V. PHOTONIC FOCK SPACE

We shall now demonstrate that the perturbation expansion indicated above can be performed in a routine way by going to the *photonic Fock space*. A single perturbation (10) takes the state vector into a Fock space, where the number of photons is no longer constant, as illustrated by the diagrams below.

To demonstrate the evaluation rules, we consider again the single-photon exchange.



Restricting ourselves to a specific time ordering, the potential (18) becomes

$$V_{\rm sp}(E_0) = \frac{e^2}{4\pi r_{12}} + \int_0^\infty \frac{f_C(k)\,{\rm d}k}{E_0 - \varepsilon_r - \varepsilon_u \mp (k - {\rm i}\eta)} \tag{31}$$

Expanding $\sin(kr_{12}/r_{12})$ in terms of radial Bessel functions and vector spherical harmonics, this can be expressed in terms of products of single-electron operators

$$V_{\rm sp}(E_0) = \frac{e^2}{4\pi r_{12}} + \frac{V^l(kr_1)\cdot V^l(kr_2)}{E_0 - \varepsilon_r - \varepsilon_u \mp (k - {\rm i}\eta)} \tag{32}$$

summed over l and k.

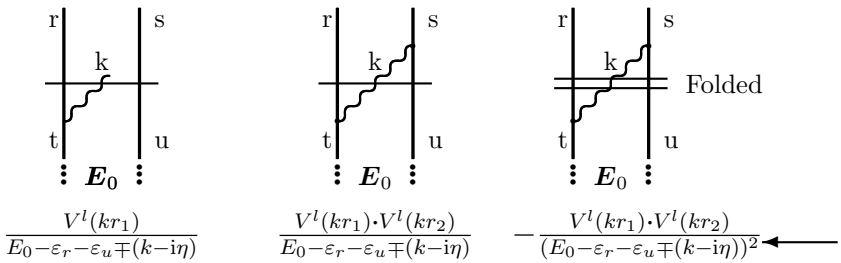
The perturbation is now

$$H' = \frac{e^2}{4\pi r_{12}} + V^l(kr_1) + V^l(kr_2) \tag{33}$$

and this leads to the *photonic Fock-space Bloch equation* for the covariant wave operator

$$[\Omega^{\rm Cov}, H_0^{\rm Fock}]P = (H'\Omega^{\rm Cov} - \Omega^{\rm Cov}\, V_{\rm eff}^{\rm Cov})P \tag{34}$$

where $H_0^{\rm Fock}$ is the zeroth-order (model) Hamiltonian, including the photon field. When the first perturbation $V^l(kr_1)$ is applied, the commutator yields—as in the standard MBPT procedure—an energy denominator, leading to the expression given under the first diagram below. Applying the second perturbation, leads after contraction and summing over l and k, to the complete Breit interaction (32), indicated by the second diagram. In the photonic Bloch equation (34) there is also a folded term, $-\Omega\, V_{\rm eff}$, which diagrammatically corresponds to a negative term with double denominator, as indicated in the last diagram below. This double denominator corresponds to the *energy derivative* of the potential. This leads to the second-order expression (28) above.



Mixing the retarded perturbations with the instantaneous Coulomb interaction (33), leads to the type of diagrams indicated in Fig. 4. The same procedure can, in principle, be used in higher orders with several uncontracted photons. This would then represent the full field-theoretical interaction between the electrons.

The consequence is that solving the Bloch equation in photonic Fock space, using the standard evaluation rules, leads to a fully covariant MBPT/CCA procedure with all kinds of relativistic and QED effects.

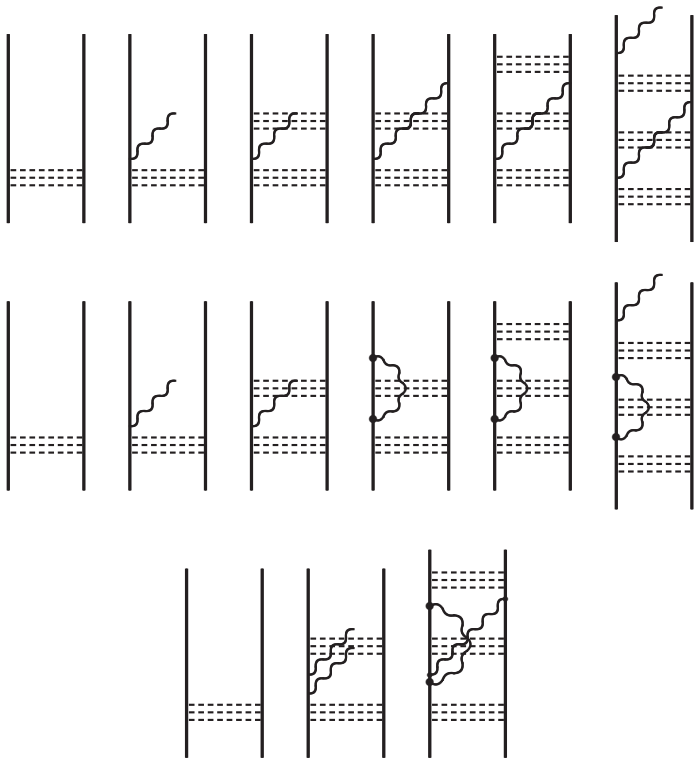


FIG. 4: Illustration of the perturbative procedure in the photonic Fock space, the first row with a single retarded photon between the electrons and the second row with a self-energy interaction, in both cases including correlation. The last row illustrates the procedure with two simultaneous, uncontracted photons, which would lead to a two-photon irreducible diagram. For the time being is not feasible to handle this kind of effect numerically.

VI. NUMERICAL RESULTS

The procedure indicated above has been applied to the ground and first excited states of He-like neon, and some result are shown in Figs 5 and 6. The results show clearly that that for light systems the first-order QED effect with correlation is considerable larger than the effect of the second-order effect with two retarded photons. As mentioned, the effect of two retarded, irreducible photons with correlation cannot presently be evaluated. On the other hand, it is possible to consider retarded reducible photons as well¡ as one retarded and one instantaneous Breit interaction (with correlation), which would represent most of the Breit-Breit interaction.

VII. SUMMARY AND OUTLOOK

A relativistically covariant MBPT/CCA procedure has been constructed, based upon the Covariant-Evolution-Operator/Green's-Operator technique. The procedure leads, in principle, to all kinds of relativistic and QED effects, and it has been demonstrated that it approaches in the two-particle case to the full Bethe-Salpeter equation, which confirms the covariance of the procedure.

The perturbative procedure is based upon Rayleigh-Scbrödinger perturbation theory, which makes the procedure size extensive and fully compatible with non-relativistic linked-diagram and coupled-cluster procedures.

By going to the photonic Fock space, the evaluation rules are essentially identical to those of standard non-relativistic MBPT/CC procedures.

The calculations presented will primarily be complemented by including virtual-pair and radiative effects. Further on, the intention is to apply the technique to quasi-degenerate fine-structure levels, thereby complementing the second-order calculation previously performed [17].

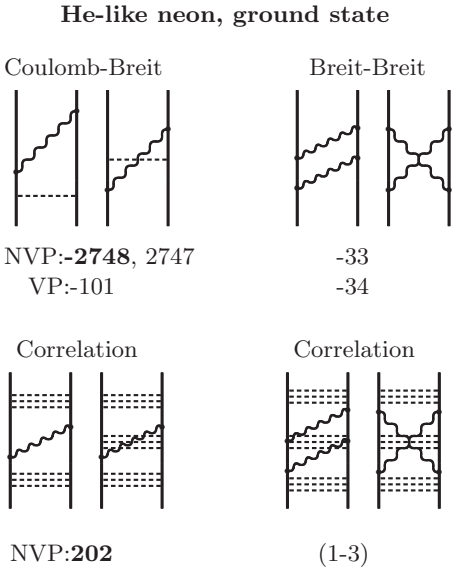


FIG. 5: Numerical results for the ground state of He-like neon. NVP=No-virtual paris, VP=virtual pairs. The numbers in bold face are from the current work, and the remaining numbers from ref. [20]. Numbers in brackets are estimated. Radiative effects are not included.

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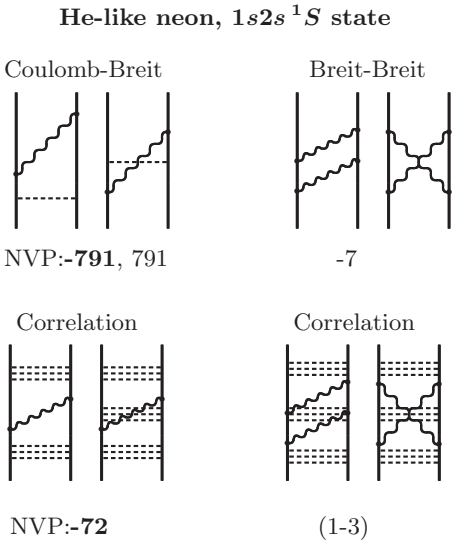

FIG. 6: Same as in Fig. 5 for the first excited state of He-like neon. The non-bold-face numbers are taken from ref. [21].

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[] This is not in accordance with the standard quantum-mechanical model and leads to some problem with the interpretation, as discussed by various authors [22–25].