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RESEARCH ARTICLE

Development of Many-Body Perturbation Theory

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The development of standard MBPT for single-reference and multi-reference cases is reviewed, and its extension to the relativistic case in the form of the Dirac-Coulomb-Breit (DCB) approximation is described. The latter scheme is non-covariant, and the recent development of a fully covariant MBPT scheme is discussed. This is based upon a new scheme for quantum-electrodynamical (QED) calculations, the covariant-evolution-operator method, which is combined with standard MBPT. This scheme is fully compatible with the relativistically covariant Bethe-Salpeter equation. Some numerical results of the new scheme are given.

Keywords: Perturbation theory; Quantum-electrodynamics; Electron correlation; Relativistic covariance; Evolution operator

1. Introduction

What is traditionally understood as *Many-Body Perturbation Theory* (MBPT) is a systematic treatment of many-body systems beyond standard low-order perturbation theory [1]. This is normally based upon the diagrammatic formulation of Rayleigh-Schrödinger (RS) perturbation expansion, which can be generated from the famous equation of Claude Bloch from 1958 [2]. This perturbation contains certain non-linear terms, and it was argued by Brueckner [3] that these terms must cancel for physical reasons. This led to the *linked-diagram* or *linked-cluster expansion*, which Brueckner proved to some low orders. Later this was proved to all orders by Goldstone [4]. In expressing the perturbations in terms of Feynman-like diagrams, only so-called linked diagrams survive.

The alternative way of treating many-body systems is the self-consistent-field methods of multi-configurational Hartree-Fock (MCHF) and Dirac-Fock (MCDF) type. We shall not consider these methods here, but refer the reader to the recent book by Grant [5].

The Brueckner-Goldstone scheme was primarily used in nuclear physics. In the 1960's it was introduced and applied in atomic physics by Kelly [6]. It was around the same time also applied on various atomic problems by Sandars [7].

The treatment of Brueckner and Goldstone was limited to a degenerate model space, where all unperturbed states under consideration have the same energy. This was extended to the non-degenerate (quasi-degenerate) case by Brandow [8] by using a double perturbation expansion and later in a more direct way by Lindgren, using a generalization of the original Bloch equation [9]. This has been found to be a good basis for many MBPT applications in atomic and molecular physics.

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Originally, the Bloch equation was expanded order by order, the problem then being that the number of terms or diagrams increases very rapidly with the order of perturbation. The situation becomes virtually impossible to handle beyond third order for a closed-shell system and even earlier for general open-shell systems.

Later, so-called *all-order methods* were developed, where certain effects, such as the *pair correlation*, could conveniently be generated to arbitrary order by an iterative process. This is more or less equivalent to the pair-correlation procedures developed early by Sinanŏglu, Nesbet, and others (see, for instance, review article by Kutzelnigg [10] and Lindgren-Morrison [1, section 15.5]).

More complete computational methods for this kind of calculations were developed at the Gothenburg and Notre Dame groups, and particularly by the latter systematically applied to various atomic systems [11].

A more efficient all-order procedure is the *Coupled-Cluster Approach* (CCA), first developed in nuclear physics and introduced into quantum chemistry by Čižek [12] already in 1965. However, it was not until the late 1970's and early 1980's that this technique was more widely used. Nowadays, this is the dominating computational procedure in quantum chemistry. Several articles in this issue are devoted particularly to the coupled-cluster procedure, and therefore I shall not go into this method in any detail here.

Relativistic many-body procedures have been developed, based upon the so-called Dirac-Coulomb-Breit or No-Virtual-Pair Approximation. This works well for many applications, but it is not relativistically covariant, since effects due to retardation of the electromagnetic interaction as well as the existence of negative energy states are omitted. The latter effects are, together with the so-called radiative effects (vacuum polarization, self energy, vertex correction), conventionally referred to as quantum-electrodynamical (QED) effects.

Several numerical methods have been developed for evaluating QED effects. Most frequently used is the S-matrix formulation, and more recently two more versatile methods have appeared, the Two-times Green's function method, developed by the St Petersburg group [13] and the Covariant-Evolution-Operator (CEO) method, developed by the Gothenburg group [14].

The existing methods for QED calculations are for practical reasons limited to two-photon exchange, which implies that the electron correlation can be only partly included. Recently, we have in Gothenburg developed a fully covariant relativistic procedure that is a combination of the standard MBPT and the CEO many-body procedure for QED calculations. This can, in principle, carry the electron correlation and QED effects to arbitrary order, an expansion that is equivalent to the full Bethe-Salpeter equation.

The work in our group in Gothenburg has been carried out in close contact with the QTP in Florida. The contact started when the author attended a summer school on the Sanibel Island in 1971 and learned basic perturbation theory from the lectures of Per-Olov Löwdin. The progress made in our group has subsequently been reported at several Sanibel conferences.

In the following we shall here first summarize the development of the standard many-body perturbation theory—non-relativistically as well as relativistically—and later turn in to the recent development of the covariant MBPT.

2. Standard many-body perturbation theory

2.1. *Degenerate case*

We consider first the simple case of a nondegenerate system with the Schrödinger equation

$$H|\Psi\rangle = E|\Psi\rangle \tag{1}$$

where H is the non-relativistic N-body Hamiltonian[1]

$$H = \sum_{i=1}^{N} \left(\tfrac{1}{2}\,\nabla^2 + v_{\rm ext}\right)_i + \sum_{i<j}^{N} \frac{e^2}{4\pi r_{ij}} \tag{2}$$

and $v_{\rm ext}$ is the external (normally nuclear) field.

The Schrödinger equation can be reexpressed as

$$(E_0 - H_0)|\Psi\rangle = (V - \Delta E)|\Psi\rangle \tag{3}$$

with the partitioning

$$H = H_0 + V\,; \qquad E = E_0 + \Delta E \tag{4}$$

We start the perturbation expansion from a *model function*, satisfying the equation, $H_0|\Psi_0\rangle = E_0|\Psi_0\rangle$. Using intermediate normalization, $\langle\Psi|\Psi_0\rangle = \langle\Psi_0|\Psi_0\rangle = 1$, the equation (3) can be expressed

$$(E_0 - H_0)|\Psi\rangle = V|\Psi\rangle - |\Psi\rangle\langle\Psi_0|V|\Psi\rangle \tag{5}$$

which is equivalent to the original Bloch equation [2].

With the order-by-order expansion

$$|\Psi\rangle = |\Psi_0\rangle + |\Psi^{(1)}\rangle + |\Psi^{(2)}\rangle + \cdots \tag{6}$$

this leads to the Rayleigh-Schrödinger expansion,

$$\begin{aligned} |\Psi^{(1)}\rangle &= V|\Psi_0\rangle - |\Psi_0\rangle\langle\Psi_0|V|\Psi_0\rangle \\ |\Psi^{(2)}\rangle &= V|\Psi^{(1)}\rangle - |\Psi_0\rangle\langle\Psi_0|V|\Psi^{(1)}\rangle - |\Psi^{(1)}\rangle\langle\Psi_0|V|\Psi_0\rangle \\ &\text{etc.} \end{aligned} \tag{7}$$

The formulation presented here works also when several unperturbed states are degenerate with the same unperturbed energy E_0 and there are no closely-lying unperturbed states.

2.2. *Quasi-degenerate case*

The situation is more challenging when there are several unperturbed states close in energy, referred to as the *quasi-degenerate* situation. Then standard perturbation

[1]We use here natural or relativistic units: $c = \hbar = m_e = \epsilon_0 = 1$, $e^2 = 4\pi\alpha$, α being the fine-structure constant.

expansion can encounter great convergence problems. A well-known example is the relativistic calculation of the fine-structure levels of heliumlike ions. For light ions the unperturbed states $2p_{1/2}$ and $2p_{3/2}$ are very close in energy, and starting from only one of them can lead to serious problems [11].

In order to handle the general quasi-degenerate situation, a different approach is needed. We consider now a *group of target states*, $|\Psi^a\rangle$, satisfying the Schrödinger equations

$$H|\Psi^a\rangle = E^a|\Psi^a\rangle \tag{8}$$

The perturbation expansion starts from one model state $|\Psi_0^a\rangle$ for each target state, and in the *intermediate normalization* this is the projection of the target states on the model space

$$|\Psi_0^a\rangle = P|\Psi^a\rangle \tag{9}$$

We introduce the *wave operator*, Ω, transforming the model states back to the target states

$$|\Psi^\alpha\rangle = \Omega|\Psi_0^\alpha\rangle \tag{10}$$

This operator is in our formalism assumed to be the same for *all* states under consideration.

With the partitioning (4) we can derive the form of an *effective Hamiltonian* in intermediate normalization

$$H_{\text{eff}} = PH\Omega P = PH_0P + PV\Omega P \tag{11}$$

satisfying the secular equation

$$H_{\text{eff}}\Psi_0^a = E^a\Psi_0^a \tag{12}$$

This implies that the target energies are the eigenvalues of the effective Hamiltonian, operating only in the model space, and the model states are the corresponding eigenvectors.

The wave operator now satisfies a *generalized Bloch equation* [9]

$$\boxed{\big[\Omega, H_0\big]P = \Big(V\Omega - \Omega V_{\text{eff}}\Big)P} \tag{13}$$

where V_{eff} is the *effective interaction*, defined by

$$H_{\text{eff}} = PH_0P + V_{\text{eff}} \tag{14}$$

and in intermediate normalization $V_{\text{eff}} = PV\Omega V$.

The generalized Bloch equation leads to a corresponding generalized Rayleigh-Schrödinger perturbation expansion. The corresponding linked-diagram expansion can be derived from the formula

$$\boxed{\big[\Omega, H_0\big]P = \Big[\big(V\Omega - \Omega V_{\text{eff}}\big)P\Big]_{\text{linked}}} \tag{15}$$

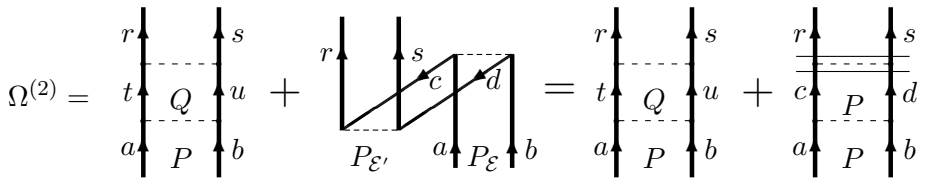

Figure 1. Diagrammatic representation of the second-order equation (16). The heavy vertical lines represent electron orbitals and propagators in the *Furry picture*. The second diagram is the "folded" diagram, which has a double denominator, associated with the last interaction. In the last diagram this is drawn straight, and the double denominator is represented by a double bar.

implying that only linked diagrams are to be retained. The last term represents here the so-called *folded diagrams*, introduced by Brandow [8].

Expansion of the Bloch equation (15) leads in lowest orders to ($Q = 1 - P$)

$$\begin{cases} \big[\Omega^{(1)}, H_0\big]P = VP - PVP = QVP \\ \big[\Omega^{(2)}, H_0\big]P = Q\big(V\Omega^{(1)} - \Omega^{(1)}V_{\text{eff}}^{(1)}\big)_{\text{linked}}P \end{cases} \tag{16}$$

The second-order equation is illustrated in Fig. 1. The single-electron orbitals are here generated in the potential of the nucleus (or some other external potential)—known as the *Furry picture*. The last diagram is the *folded diagram* that represents the contribution due to an intermediate state in the model space, *model-space contribution* (MSC). Such a state leads to a *(quasi)singularity* that is automatically eliminated by the Bloch equation.

Once the wave operator is determined to the desired accuracy, the corresponding wave functions are obtained from the definition (10). In the general case the model functions are not known in advance, but they can be obtained by means of the secular equation (12).

The linked-diagram expansion for the open-shell case (Eq. 15) holds provided the model space is *complete*, i.e., contains all configurations that can be formed by the valence electrons. It can be shown to hold also for an incomplete model space, if the intermediate-normalization condition is abandoned, as demonstrated by Mukherjee [15].

With the *"extended"* model space described here the quasi-degenerate problem can normally be handled without problem. This is illustrated, for instance, in the case of the fine structure of light heliumlike ions, mentioned above. With this technique the calculations converge nicely for all nuclear charges [16].

We have assumed here that we work in a scheme known as *multi-reference*, implying that the wave operator is the same for all states belonging to the model space. In such a case convergence problems will appear, if a state under consideration will cross a state not belonging to the model space, as the perturbation is adiabatically turned on. A well-known example is here the Be atom, if the model space is chosen to contain the configurations $1s^2\,2s^2$ and $1s^2\,2p^2$. This problem is much more pronounced in molecular applications than in atomic ones.

2.3. *All-order approaches*

By means of second quantization the wave operator can be separated into one-, two-, ... body effects

$$\Omega = 1 + \Omega_1 + \Omega_2 + \cdots \tag{17}$$

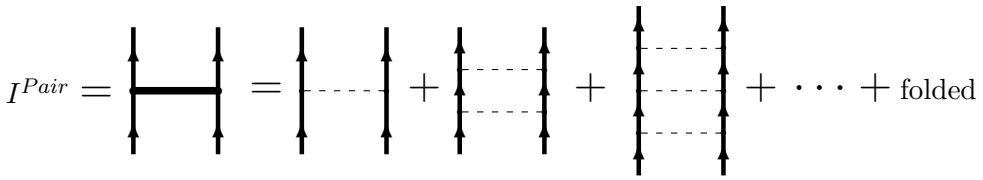

Figure 2. Expansion of the all order pair function (20).

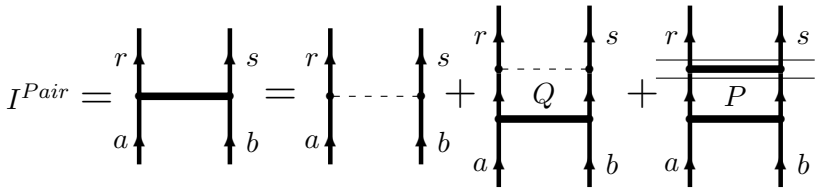

Figure 3. Graphical representation of the self-consistent pair equation (19). The last diagram represents the "folded" diagram, drawn in analogy with that in Fig. 1 (right).

This leads to the corresponding partitioning of the following Bloch equation

$$\big[\Omega_n, H_0\big]P = \big(V\Omega - \Omega V_{\rm eff}\big)_{{\rm linked},n}P \tag{18}$$

and solving a number of these coupled sub-equations iteratively, yields the corresponding effects essentially to all orders. This is known as the *all-order perturbation approach*, which is frequently employed.

Including only double excitations (pair correlation), $\Omega \approx 1+\Omega_2$, leads to the *pair equation*

$$\big[\Omega_2, H_0\big]P = Q\Big(V(1+\Omega_2) - \Omega_2 V_{\rm eff}\Big)_{{\rm linked},2}P \tag{19}$$

This can also be expressed

$$\Omega_2 P_{\mathcal{E}} = \Gamma_Q(\mathcal{E}) I^{\rm Pair} P_{\mathcal{E}} \tag{20}$$

operating on a part of the model space with energy $\mathcal{E}$. Here,

$$\Gamma_Q(\mathcal{E}) = \frac{Q}{\mathcal{E} - H_0} \tag{21}$$

is the reduced resolvent and $I^{\rm Pair}$ is a ladder of Coulomb interactions, including the folded terms, illustrated in Fig. 2. This can also be graphically expressed in the form of a Dyson equation, as shown in Fig. 3.

An even more effective way of treating electron correlation is the *coupled-cluster approach* or *exponential Ansatz*, which we shall not consider further here (see, other articles in this issue and the recent book, edited by Čársky et al. [**?**]).

2.4. *Relativistic MBPT*

For relativistic many-body calculations a natural starting point is to replace the Schrödinger single-electron Hamiltonian in the Hamiltonian (2) by the corresponding Dirac operator

$$h_D = \boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}} + \beta + v_{\rm ext} \tag{22}$$

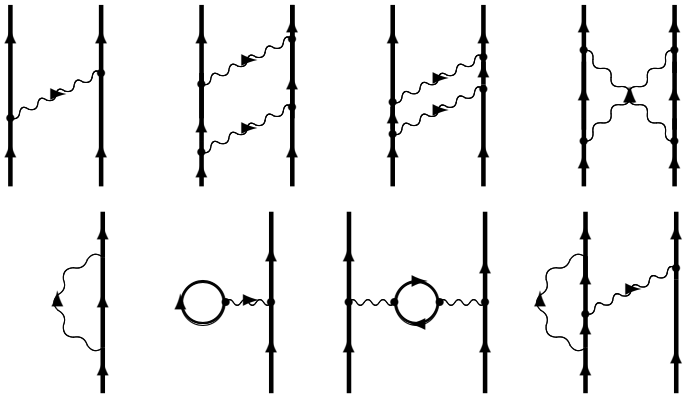

Figure 4. Some low-order non-radiative (upper line) and radiative (lower line) "QED effects". These diagrams are *Feynman diagrams*, and the heavy lines represent particle as well as hole or anti-particle states in the *Furry picture*. The wavy lines represent the covariant photon exchange. The second diagram is, when the intermediate states are *particle* states, *reducible*, since it can be separated into two single-photon-exchange diagrams, while all the remaining diagrams are *irreducible*.

Such an operator would not be bound from below due to the negative-energy eigenstates of the Dirac operator. In order to prevent these from entering, a projection operator Λ_+ can formally be introduced. Including also the *instantaneous Breit interaction*

$$H_B = -\frac{e^2}{8\pi} \sum_{i<j} \Big[\frac{\alpha_i \cdot \alpha_j}{r_{ij}} + \frac{(\alpha_i \cdot r_{ij})(\alpha_j \cdot r_{ij})}{r_{ij}^3} \Big] \tag{23}$$

this leads to the *projected Dirac-Coulomb-Breit approximation*, first formulated by Sucher [17],

$$H = \Lambda_+ \Big[\sum_{i=1}^{N} h_D(i) + \sum_{i<j}^{N} \frac{e^2}{4\pi r_{ij}} + H_B \Big] \Lambda_+ \tag{24}$$

This is also known as the *No-Virtual-Pair Approximation* (NVPA). In many self-consistent calculations of Dirac-Fock type no explicit projection operators are used, but the boundary conditions used have the effect of eliminating the negative-energy states.

Effects beyond the NVPA are conventionally referred to as *QED effects*, and the lowest-order diagrams are depicted in Fig. 4. The first row represents so-called *non-radiative effects*, or Araki-Sucher effects, and the second row *radiative effects* (self energy, vacuum polarization and vertex correction).

2.5. *Implementation*

The MBPT technique is nowadays widely used in atomic and molecular physics. Here, I will concentrate on atomic applications, since molecular applications will be covered in other articles of this issue.

The MBPT procedure was first applied to electronic systems by Kelly in the 1960's, using a basis set of analytical functions, nowadays frequently used in molecular applications. Later, accurate numerical approaches were developed for atomic applications. One of the first application was made by Morrison and Rajnak, using numerical one- and two-particle functions [18]. This technique was subsequently further developed by Morrison together with the Gothenburg group and applied

to fine- and hyperfine-structure problems [1]. An all-order single-particle program was developed by Lindgren and Garpman et al. [19] and an all-order pair program by Ann-Marie Mårtensson [20], a procedure that was further developed into a coupled-cluster procedure by Salomonson [21, 22]. A relativistic pair program was later developed by Eva Lindroth [23]. The numerical technique was further refined by Salomonson and Öster by introducing a "discretization technique" [24]. This technique has subsequently been applied in various relativistic and non-relativistic many-body calculations by the Gothenburg group.

An all-order relativistic pair program, based upon the Dirac-Coulomb-Breit Hamiltonian (24) was also developed by Johnson et al. at Notre Dame, using a numerical spline technique [25], and applied to numerous atomic systems [11, 26].

The atomic many-body perturbation technique has also been frequently applied to other problem than energy calculations, such as the photo-ionization process [**? ?**].

3. Covariant many-body procedure

3.1. *Time-dependent perturbation theory*

In developing a covariant many-body procedure it is necessary to consider the time dependence of the perturbation. It is convenient to use the *interaction picture* (IP), where the state vectors and operators are related to those in the Schrödinger picture (SP) by

$$|\chi_{\rm I}(t)\rangle = {\rm e}^{{\rm i}H_0 t}\,|\chi_{\rm S}(t)\rangle; \qquad V_{\rm I}(t) = {\rm e}^{{\rm i}H_0 t}\,V\,{\rm e}^{-{\rm i}H_0 t} \tag{25}$$

The time-dependent Schrödinger equation then becomes

$${\rm i}\frac{\partial}{\partial t}|\chi_{\rm I}(t)\rangle = V_{\rm I}(t)\,|\chi_{\rm I}(t)\rangle \tag{26}$$

The *time-evolution operator* in IP, $U(t,t_0)$, is defined by[1]

$$|\chi(t)\rangle = U(t,t_0)\,|\chi(t_0)\rangle \qquad (t>t_0) \tag{27}$$

and it satisfies the differential equation

$${\rm i}\frac{\partial}{\partial t}U(t,t_0) = V(t)\,U(t,t_0) \tag{28}$$

This leads to the expansion

$$U_\gamma(t,t_0) = \sum_{n=0}^{\infty}\frac{(-{\rm i})^n}{n!}\int_{t_0}^{t}{\rm d}t_1\ldots\int_{t_0}^{t}{\rm d}t_n\,T\big[V(t_1)\ldots V(t_n)\big]\,{\rm e}^{-\gamma(|t_1|+|t_2|\ldots+|t_n|)} \tag{29}$$

where T is the *time-ordering operator* and γ is an *adiabatic damping factor*.

For finite times the evolution operator is non-covariant. Setting $t=\infty$ and $t_0=-\infty$, leads to the S-matrix

$$S = U(\infty,-\infty) \tag{30}$$

[1]In the following we shall leave out the subscript "I".

which is relativistically covariant.

The perturbation above is represented by the interaction between an electron and the radiation fields

$$V(t) = \int \mathrm{d}^3x\, \mathcal{H}(t,\boldsymbol{x})\,; \qquad \mathcal{H}(x) = -e\hat{\psi}^\dagger(x)\alpha^\mu A_\mu(x)\hat{\psi}(x) \tag{31}$$

where $x = (t,\boldsymbol{x})$ is the four-dimensional space-time coordinate and $\hat{\psi}(x)$, $\hat{\psi}^\dagger(x)$ and A_μ are the electron-field and the photon-field operators, respectively. The expansion (29) then becomes

$$U(t,t_0) = \sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n}{n!} \int_{t_0}^{t} \mathrm{d}^4x_1 \ldots \int_{t_0}^{t} \mathrm{d}^4x_n\, T\big[\mathcal{H}(x_1)\ldots\mathcal{H}(x_n)\big]\, \mathrm{e}^{-\gamma(|t_1|+|t_2|\ldots+|t_n|)} \tag{32}$$

Here, the perturbation operates in the *extended photonic Fock space*, where the number of photons is no longer constant. The exchange of a single (virtual) photon is represented by two perturbations of this kind. In Fig. 5 we show the Feynman diagram representing a single-photon exchange between the electrons. This contains two time orderings, as indicated by the two time-ordered diagrams.

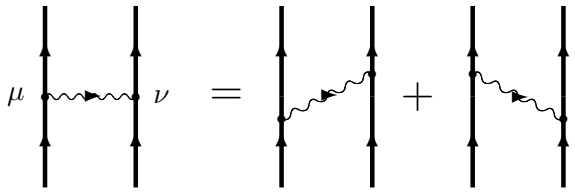

Figure 5. The Feynman representation of the exchange of a single, virtual photon between two electrons. This contains two time-orderings.

3.2. *Covariant many-body Hamiltonian*

The Dirac-Coulomb-Breit relativistic Hamiltonian (24) is not relativistically covariant, since only positive-energy states are considered. In order to be able to treat electron correlation and QED effects on the same footing, it is necessary to start from a Hamiltonian that is fully covariant. This can be achieved by replacing the electron-electron interaction by the covariant interaction (31). We want here to use the Coulomb gauge, and therefore we separate the interaction into the Coulomb interaction and the transverse-photon interaction. In second quantization this leads to the covariant many-body Hamiltonian

$$\begin{aligned} H_{\mathrm{Cov}} &= H_0 - \int \mathrm{d}^3\boldsymbol{x}\, \hat{\psi}^\dagger(x) e\alpha^\mu A_\mu(x)\hat{\psi}(x) \\ &\quad + \frac{1}{2}\iint \mathrm{d}^3\boldsymbol{x}_1\, \mathrm{d}^3\boldsymbol{x}_2\, \hat{\psi}^\dagger(x_1)\, \hat{\psi}^\dagger(x_2) \frac{e^2}{4\pi r_{12}}\, \hat{\psi}(x_2)\, \hat{\psi}(x_1) \\ H_0 &= \int \mathrm{d}^3\boldsymbol{x}\, \hat{\psi}^\dagger(x)\Big(\boldsymbol{\alpha}\cdot\hat{\boldsymbol{p}} + \beta + v_{\mathrm{ext}}\Big)\hat{\psi}(x) + H_{\mathrm{Rad}} \end{aligned} \tag{33}$$

The first part of the perturbation contains the transverse-photon interaction and corresponds to the Breit interaction in the DCB Hamiltonian (24), and the follow-

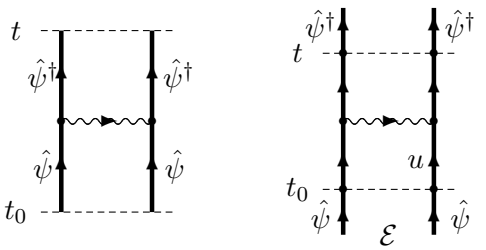

Figure 6. Comparison between the standard and the covariant evolution operator for single-photon exchange. In the latter there are electron propagators on the in- and outgoing lines, implying that they can represent particle or hole with time running both ways.

ing term represents the Coulomb interaction. $H_{\rm Rad}$ in the zeroth-order Hamiltonian is the Hamiltonian of the radiation field, which has to be included, since the number of photons is no longer constant in this formalism.

3.3. *Covariant evolution operator. Green's operator. Connection to MBPT*

In order to make the evolution operator relativistically covariant, we must allow time to run also *backwards* in the negative direction, corresponding to the propagation of *hole or antiparticle states* with negative energy. This can be achieved by inserting electron propagators on the free lines, as shown in Fig. 6. This leads to the *covariant evolution operator* (CEO), introduced by Lindgren, Salomonson and coworkers [14].

The covariant evolution operator contains *singularities* in higher orders, when there is an intermediate state in the model space (c.f. Fig. 3). Eliminating these singularities leads to what we have referred to as the *Green's operator*, since this object is quite analogous to the *Green's function*. This operator plays a central role in the present formalism.

We define the Green's operator, $\mathcal{G}(t,-\infty)$, by

$$\boxed{U(t,-\infty)P = \mathcal{G}(t,-\infty)\cdot PU(0,-\infty)P} \tag{34}$$

where the heavy dot implies that the operator to the left does not operate beyond the dot. The Green's operator for $t=0$ corresponds to the standard wave operator in MBPT (10) and can be regarded as its extension to the covariant formalism,

$$\boxed{\Omega \Rightarrow \mathcal{G}(0,-\infty)} \tag{35}$$

For the moment neglecting virtual pairs, the covariant wave operator satisfies in the lowest orders the equations

$$\begin{cases} \Omega^{(1)}P_{\mathcal{E}} = \Gamma_Q(\mathcal{E})V(\mathcal{E})P_{\mathcal{E}} \\ \Omega^{(2)}P_{\mathcal{E}} = \Gamma_Q(\mathcal{E})\Big[V(\mathcal{E})\Omega^{(1)} - \Omega^{(1)}V_{\rm eff}^{(1)} + \frac{\delta V(\mathcal{E})}{\delta\mathcal{E}}\,V_{\rm eff}^{(1)}\Big]_{\rm linked}P_{\mathcal{E}} \end{cases} \tag{36}$$

The second term on the rhs of the second equation is identical to the folded term of MBPT (Eq. 16), and the last term is an additional contribution from the intermediate model-space state due to the energy dependence of the potential. This

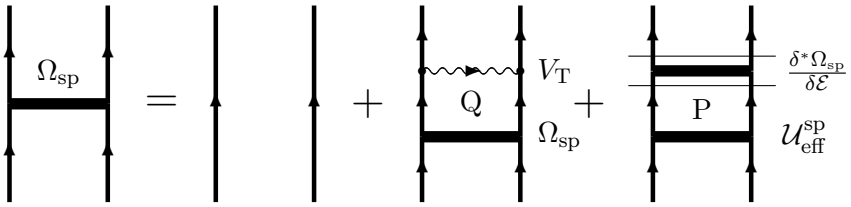

Figure 7. Graphical representation of the single-photon Bloch equation (38). This represents the first step towards the full Bethe-Salpeter equation.

Table 1. Comparison in the ground state of some heliumlike ions between two-photon Coulomb-Breit (unretarded no-pair, retarded no-pair, and virtual pairs) and correspondingly WITH electron correlation, beyond two photons (in μH).

	Two-photon Coul-Breit			Beyond Two-phot. Coul-Breit		
Z	Unretarded	Retarded	Virt.pairs	Unretarded	Retarded	Virt.pairs
6	-1055	32	-10	137	-17	2.7
10	-2871	122	-46	223	-40	7.3
14	-5517	293	-122	301	-68	13
18	-8949	553	-248	372	-100	21
30	-23632	1909	-1010	553	-210	46
41	-43521	3904	-2435	688	-322	71

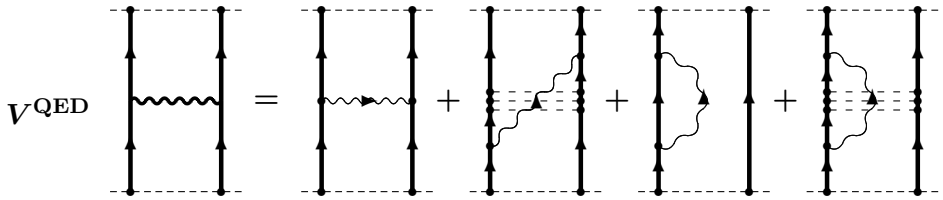

Figure 8. Feynman diagram representing the "QED potential", containing also radiative QED effects.

equation can also be expressed

$$\Omega^{(2)}_{\rm Cov} P_{\mathcal{E}} = \left[\Gamma_Q(\mathcal{E})\, V(\mathcal{E})\, \Omega^{(1)} + \frac{\delta\Omega^{(1)}}{\delta\mathcal{E}}\, V^{(1)}_{\rm eff} \right]_{\rm linked} P_{\mathcal{E}} \tag{37}$$

Generalizing this to all orders, leads to the Bloch equation

$$\Omega P_{\mathcal{E}} = \left[1 + \Gamma_Q(\mathcal{E}) V(\mathcal{E})\, \Omega + \frac{\delta^*\Omega}{\delta\mathcal{E}}\, V_{\rm eff} \right] P_{\mathcal{E}} \tag{38}$$

In the last folded term we have introduced the symbol δ^*, implying that *only the last interaction, including the associated resolvent, is differentiated.* This equation is illustrated in Fig. 7. In the presence of virtual pairs, we can modify the potential by a Coulomb interaction, so that in- and outgoing states of the modified potential are all positive-energy states.

The procedure described so far contains only the so-called non-radiative QED effects (top row in Fig. 4). Some radiative effects can be included into the potential, as illustrate in Fig. 8. This involves the exchange of a retarded photon between the electrons as well as self interaction, in both cases with and without crossing

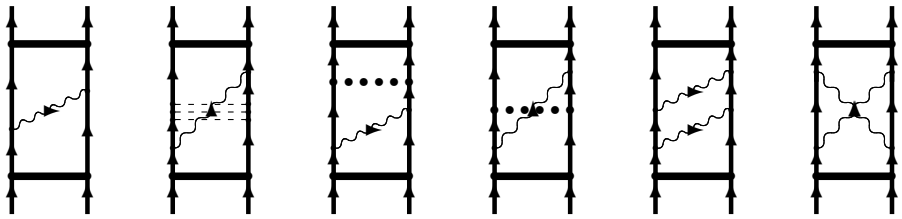

Figure 9. One- and two-photon exchange diagrams with electron correlation, represented by incoming and/or outgoing pair functions with one or several Coulomb interactions.

Coulomb interactions. In addition, vacuum-polarization effects can be included by modifying the electron and photon propagators. These modifications have not yet been implemented but seem quite feasible. This would then generate most of the QED effects.

To go further, the next step would be to include also irreducible two-photon effects (see Fig. 4). This is not feasible for the time being, but a reasonable approximation would be to replace one of the photons by the instantaneous Breit interaction (23) (see Fig. 9).

By continuing this procedure and including more and more *irreducible* interactions, this will eventually lead to the solution of the fully covariant two-particle ***Bethe-Salpeter equation***, as recently demonstrated by Lindgren et al. [27].

4. Implementation of the covariant procedure

The covariant form of MBPT, described here, is now being implemented at our laboratory. The first diagram in Fig. 9, corresponding to a single, retarded photon with iterated Coulomb interactions (Fig. 2) in and out, has been fully implemented—with all combinations of particles and holes. This corresponds to evaluating the corresponding QED effects with a fully correlated wave function of Hylleraas type. The second diagram with crossing Coulomb interactions is implemented in the no-pair approximation. The results are given in the second part of Table 1 and displayed in Fig. 10. These results are compared in the first part of the table with corresponding two-photon S-matrix results [28]. The results are presented in the thesis of Daniel Hedendahl [29] and will be published shortly. *This represents the first calculations ever performed beyond two-photon exchange.*

The next two diagrams in Fig. 9, which include one retarded and one unretarded Breit interaction, are also quite feasible to evaluate, while the last two—with TWO retarded interactions—are beyond reach for the time being. It should be noted, though, that the corresponding effects would be quite small. In Fig. 10 we have also indicated the (estimated) effect of doubly retarded two-photon exchange with correlation.

One important conclusion that can be drawn from our results is that ***the effect of electron correlation on the first-order QED effect is considerably larger than the second-order QED effect for light and medium-heavy elements***.

In the pipeline for us is presently to implement the radiative part of the potential in the figure 8. This will require regularization and renormalization in the Coulomb gauge, which is doable but not straightforward.

Our intention is also to apply the procedure to excited states of heliumlike ions in order to evaluate level separations, such as the fine-structure splitting. Very accurate experimental results are here available that presently have no matching

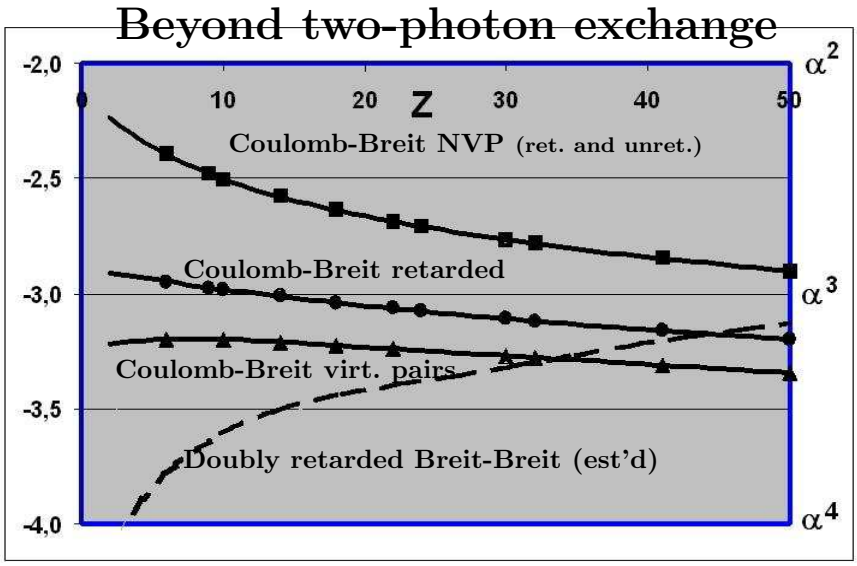

Figure 10. The Coulomb-Breit interaction with electron correlation beyond two-photon exchange, unretarded (squares), retarded (circles), and virtual pairs (triangles). Included is also the (estimated) two-photon Breit-Breit interaction with DOUBLE retardation and correlation (dashed). The values are normalized to the ionization energy. The vertical scale is logarithmic with one unit corresponding to a factor of the fine-structure constant $\alpha \approx 1/137$.

theoretical counterpart [30, 31]. In order to reach sufficient accuracy, our numerical procedure has to be further improved, a procedure that is presently under way in collaboration with the mathematical department at our university.

To what extent we will be able to realize the ambitious program indicated here, will largely depend on the economical and personal resources that we can access in the future.

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