Molecular Physics **98**, 1159-74 (2000)

Can MBPT and QED be merged in a systematic way?

Ingvar Lindgren
Department of Physics, Chalmers University of Technology
and Göteborg University, Göteborg, Sweden

Abstract

The possibilities of merging QED with the standard many-body perturbation theory (MBPT) for atomic systems in a rigorous and systematic way are analysed. Time-dependent MBPT, based on the time-evolution operator, a technique well developed particularly in nuclear theory, is used and somewhat reformulated to be consistent with the covariant QED formalism. An effective QED Hamiltonian, free from singularities, is constructed. The procedure can be applied to degenerate and quasi-degenerate systems (extended model space), which is not possible with the standard QED technique based upon the S-matrix formulation. To include in the model space closely lying energy levels, such as fine-structure levels, can have a drastic effect on the convergence rate. The electron-electron interaction is investigated in detail, and it is shown that it can be separated into irreducible multi-photon interactions, which in principle can be iterated as in standard MBPT. Singularities do not appear, and a simple procedure for evaluating residual finite contributions is described. Comparison is made with the closely related Green's-function technique. The procedure is presently being tested on the fine-structure levels of He-like ions, the results of which will be published separately.

1 Introduction

Essentially there are two approaches to atomic many-body theory, the self-consistent and the perturbative. The two approaches are complementary, and each has merits and shortcomings. The self-consistent technique of multi-configuration Hartree-Fock (MCHF) has been developed to a high degree of sophistication, particularly by Charlotte Froese-Fischer and her associates, and the technique has now become a general and efficient tool, which can be used also by non-specialists. Our group in Göteborg has been working mainly with the alternative perturbative approach, although also non-perturbative methods (coupled-cluster approach) have been developed from this ansatz.

During the last decade there has been increasing interest in relativistic and quantum-electrodynamical (QED) calculations on heavy and highly charged systems, due mainly to the advent of new experimental techniques, such as storage rings and ion traps, which make it possible to study such systems with high accuracy. For instance, the atomic g-factor for hydrogen-like carbon has recently been measured using the ion-trap technique by the Mainz group with an accuracy of $1 : 10^9$ [1], verifying previous theoretical calculations from our group of corresponding accuracy [2, 3].

In principle, it is possible to base atomic-QED calculations entirely upon QED, and this

is the technique normally employed on simple systems. This procedure, however, is limited to systems with only a few electrons. Another disadvantage with this approach is that the QED calculations become very cumbersome already at second order and will be almost prohibited beyond that order in the foreseeable future. For many systems, particularly lighter ones, where the Coulomb interaction dominates, the convergence of a perturbative approach is very slow. In MBPT, iterative and non-perturbative approaches have been developed, which make it possible to include the dominating perturbations essentially to all orders of perturbation theory. These approaches have been quite successful and frequently used in atomic/molecular physics and quantum chemistry. It would be desirable to be able to include some of these iterative ideas also into QED calculations. The work presented here is an effort in this direction.

It is also of interest to be able to perform QED calculations on systems with more than a few electrons. For instance, X-ray energies can now be obtained with such a high accuracy that the QED effects are clearly visible [4]. The standard procedure today for atomic-QED calculations on such systems is to perform the two calculations independently. After the MBPT or SCF calculation has been completed, a "QED correction" is added [5]. Such a procedure is satisfactory up to a certain level, but it gives no way of gradually improving the result. To go beyond that it will be necessary to merge the two approaches together in a more systematic fashion. In recent time we have made certain progress along these lines, and such a combined procedure, based upon the perturbative approach to many-body theory, will be outlined in the present paper.

Most MBPT works on general systems are based upon the *effective-Hamiltonian approach*, i.e., the solution of the secular equation [6]

$$H_{\rm eff}\Psi_0^\alpha = E^\alpha\Psi_0^\alpha \qquad (\alpha = 1, 2, \ldots d). \tag{1}$$

$H_{\rm eff}$ is here an *effective Hamiltonian*, which has the important property that although it operates only within a subspace of the Hilbert space of the system (the model space, D, of dimensionality d), it *generates the exact energies of the system*, corresponding to the parent states in the model space. In addition, the secular equation generates the *correct zeroth-order functions* (ZOF) or parent states, Ψ_0^α, which are eigenfunctions of the effective Hamiltonian in the model space. After diagonalization of the effective Hamiltonian, the full wave functions, Ψ^α, can be constructed from the ZOF's by means of the *wave operator* or *Møller operator* [7], Ω,

$$\Psi^\alpha = \Omega\Psi_0^\alpha \qquad (\alpha = 1, 2, \ldots d), \tag{2}$$

satisfying the equation

$$H\Omega = \Omega H_{\rm eff}, \tag{3}$$

where H is the Hamiltonian of the system.

The equations above can be solved in a perturbative way by expanding the wave operator order-by-order. Alternatively, the wave operator can be expanded by means of second quantization in one-, two-, ... body operators, which leads to the coupled-pair and coupled-cluster approaches [6]. The equations can then be solved in a non-perturbative way, including certain types of excitations to all orders of perturbation theory. Such approaches have been demonstrated to be quite efficient for many atomic and molecular as well as nuclear systems.

Most QED calculations performed for bound systems are based upon the S-matrix formulation of QED and the adiabatic procedure of Gell-Mann–Low [8] and Sucher [9] to eliminate the singularities. Although this procedure works well in many cases, it has several limitations. Firstly, being based on the S-matrix, the procedure can only yield matrix elements *diagonal in energy*. This implies that it cannot be applied to an *extended model*

space with several (quasi-degenerate) eigenvalues. The fine-structure levels of light elements is a good example of a quasi-degenerate case, and the inclusion of the closely lying levels in the model space can here improve the convergence rate dramatically, as was clearly demonstrated recently in a relativistic (non-QED) MBPT calculation on helium-like systems [10]. Furthermore, in the S-matrix formalism the singularities are eliminated by the adiabatic process at the end of the calculation, which makes the evaluation of the residual finite parts quite cumbersome beyond the lowest orders.

The procedure outlined in the present paper is based upon the *time-evolution operator*, $U(t, t_0)$, which evolves the state forward in time,

$$\Psi(t) = U(t, t_0)\Psi(t_0). \tag{4}$$

This is the basic tool in non-covariant perturbation theory, which has been applied in non-QED calculations for a long time [11, 12]. In the present paper this procedure will be modified to be applicable also to bound-state QED problems. This requires that the evolution operator is *generalized to include forward as well backward time evolution*, which makes it possible to adopt the *covariant Feynman approach*. It will be shown that in this way an effective QED Hamiltonian of the type (1) can be derived, applicable also to an extended model space. This Hamiltonian is *free from singularities*. The singularities are eliminated by means of a *factorization procedure*, similar to that developed in nuclear theory in the 1970's, and which leads to a generalization to degenerate and quasi-degenerate systems of the Gell-Mann–Low procedure. With the generalized form of the evolution operator the procedure is made covariant, and this is an alternative to the Sucher modification, based upon the S-matrix. Being based upon the covariant evolution operator rather than on the S-matrix, makes it applicable also to quasi-degenerate systems.

Another difference from standard time-dependent perturbation theory is that in QED also the interactions are *time dependent*, which will lead to *residual finite contributions*, when the singularities are eliminated. A simple procedure for evaluating these finite contributions is described. Since the operators involved are free from singularities, the adiabatic switching can be performed independently for each interaction, leading to exact energy conservation at each vertex.

It will also be shown that the multi-photon interaction between the electrons can be separated into *irreducible one-, two-, ... photon interactions* [13],

$$V_{21}^{\text{Irred}} = V_{21}^{(1)} + V_{21}^{(2)} + \dots \tag{5}$$

These irreducible multi-photon interactions are free from singularities and can in principle be iterated as in the standard MBPT procedure. The intermediate states between the irreducible interactions are restricted to the complementary space (outside the model space), which makes the entire procedure non-singular. Including all irreducible two-body interactions to all orders is equivalent to solving the complete *Bethe-Salpeter equation* [14]. Iterating the one-photon interaction corresponds to the *ladder approximation* of this equation. The one-photon interaction obtained here is an alternative to the so-called Mittleman potential [15].

The procedure introduced here is closely related to the two-times Green's-function technique, developed and applied by Shabaev and coworkers [16, 17, 18], and a relation between the two techniques will be shown. In a forthcoming paper the procedure will be further developed and presented together with numerical illustrations [19].

2 Time-independent many-body perturbation theory

2.1 General

In this section we shall briefly outline the time-independent MBPT as a background for the time-dependent treatments that will follow. MBPT normally starts by partitioning the Hamiltonian [6]

$$H = H_0 + H' \tag{6}$$

of the system into an unperturbed Hamiltonian,

$$H_0 = \sum_{i=1}^{N} h_S(i); \qquad h_S = -\frac{\hbar^2}{2m}\nabla^2 - \frac{\mathrm{e}^2 Z}{4\pi\epsilon_0 r} + U(r), \tag{7}$$

composed of single-particle Schrödinger Hamiltonians, h_S, and a perturbation

$$H' = \sum_{i<j=1}^{N} \frac{\mathrm{e}^2}{4\pi\epsilon_0 r_{ij}} - \sum_{i=1}^{N} U(r_i). \tag{8}$$

N is the number of electrons of the system, and U is a single-electron potential that represents (in an approximate way) the interaction from the remaining electrons. (In the following, we shall employ relativistic units $m = c = \epsilon_0 = \hbar = 1$; $\mathrm{e}^2 = 4\pi\alpha$, where α is the fine-structure constant.)

The eigenfunctions of H_0 are assumed to be known

$$H_0\Phi_i = E_i^0\Phi_i,$$

and we search the solutions of the full Schrödinger equation

$$H\Psi^\alpha = E^\alpha\Psi^\alpha.$$

The basis functions Φ_i can be expressed in terms of antisymmetrized combinations (Slater determinants) of single-electron orbitals, $\phi_i(\mathbf{x})$, which are eigenfunctions of h_S

$$h_S\,\phi_i(\mathbf{x}) = \varepsilon_i\,\phi_i(\mathbf{x}).$$

We select a sub-space (D) of dimensionality d of the complete Hilbert space of the system, called the *model space*, which is spanned by the eigenfunctions of H_0 (Slater determinants) corresponding to one or several eigenvalues. We are interested in the corresponding full wave functions, which we can express by means of a *wave operator* Ω, the same for the entire model space (2),

$$\Psi^\alpha = \Omega\Psi_0^\alpha \qquad (\alpha = 1, 2, \ldots d). \tag{9}$$

The functions Ψ_0^α, which lie in the model space, are the parent states and will be referred to as the *correct zeroth-order wave functions* (ZOF). It should be noted that these functions need in the general case not be identical to any of the basis functions Φ_i we have chosen initially.

We separate the single-electron orbitals of the atom into *core, valence* and *excited orbitals*. The core shells are filled (closed) in the model space, while the valence shells are normally unfilled (open) - but also filled shells can be treated as valence shells. The excited orbitals are unoccupied in the model space. A model space is said to be *complete*, if it contains all

determinants that can be formed from the orbitals of the valence shell(s) - in addition to the closed-shell electron core.

The wave operator satisfies the generalized Bloch equation [20, 21, 6, 22]

$$[\Omega, H_0]P = (H'\,\Omega - \Omega H'_{\rm eff})P, \tag{10}$$

where H'_{eff} is the *effective perturbation*, related to the full effective Hamiltonian by

$$H_{\rm eff} = PH_0P + H'_{\rm eff}, \tag{11}$$

P is the projection operator for the model space, and we introduce the corresponding projection operator, Q, for the complementary space

$$P + Q = 1. \tag{12}$$

Although it acts only within the model space, the effective Hamiltonian generates the exact energies of the system (1), corresponding to the parent states in the model space,

$$H_{\rm eff}\Psi_0^\alpha = E^\alpha\Psi_0^\alpha \qquad (\alpha = 1, 2, \ldots d). \tag{13}$$

In addition, the eigenfunctions of $H_{\rm eff}$ are the ZOF's. The Bloch eqn (10) can also be given a more compact form (3), without using the partitioning (6),

$$H\Omega P = \Omega H_{\rm eff}. \tag{14}$$

Assuming that the wave operator has an inverse, we can then express the effective Hamlitonian as

$$H_{\rm eff} = P\Omega^{-1}H\Omega P. \tag{15}$$

Most MBPT works are based on the so-called *intermediate normalization*, where $\langle\Psi_0^\alpha|\Psi^\alpha\rangle = 1$, which implies that

$$\Psi_0^\alpha = P\Psi^\alpha \quad \text{and} \quad P\Omega P = P \tag{16a}$$

and the effective Hamiltonian and the effective perturbation get the form

$$H_{\rm eff} = PH\Omega P \quad \text{and} \quad H'_{\rm eff} = PH'\,\Omega P \tag{16b}$$

This gives the Bloch eqn (10) the form

$$[\Omega, H_0]P = (H'\,\Omega - \Omega PH'\,\Omega)P \tag{16c}$$

By expanding the wave operator in a perturbation series, this leads to a general form of the *Rayleigh-Schrödinger perturbation expansion*, valid also for an extended model space.

In the general case the ZOF's are not known from the start. The procedure is then first to evaluate the effective Hamiltonian matrix in the model space to the desired accuracy. If there are several states in the model space of the same symmetry, the effective Hamiltonian will also have *non-diagonal elements*. Diagonalizing the matrix then yields the corresponding energies and the ZOF's. If the wave functions are needed, they can subsequently be obtained by evaluating the wave operator by means of the Bloch eqn (10) and applying (9).

The relation (16a) implies that with the intermediate normalization all contributions to Ω beyond the zeroth order lie in the Q space. It also follows in this case from the order-by-order expansion of (16c) that *all intermediate states will lie in the Q space.*

2.2 Linked-diagram theorem

It is convenient to express the operators in *second-quantized form*, i.e., for one- and two-body operators [6]

$$f = \sum_{i,j} c_i^\dagger \, \langle i|f|j\rangle \, c_j; \qquad g = \sum_{i,j,k,l} c_i^\dagger c_j^\dagger \, \langle ij|g|kl\rangle \, c_l c_k. \tag{17}$$

where $c_i^\dagger, c_i$ are *electron creation and absorption operators*, respectively, satisfying the usual anticommutation relations for fermions

$$\{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0; \qquad \{c_i^\dagger, c_j\} = \delta_{ij}. \tag{18}$$

By means of Wick's theorem the terms appearing in the perturbation expansion can then be conveniently represented by diagrams of Feynman or Goldstone type. A free line of a diagram is associated with an uncontracted creation/absorption operator, and it follows that an operator acting on the model space (to the left or to the right) can have no other free orbital lines than valence lines on that side. The diagrams of the effective Hamiltonian can have no other free lines than valence lines whatsoever (see Fig. 1). Such diagrams are said to be *closed*. A diagram which is not closed is *open*.

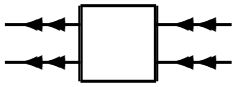
$H_{\rm eff} = 1 \; + \; P\,H_0\,P \; +$ 

Figure 1: The effective Hamiltonian is (apart from the H_0 part) represented by linked diagrams that are closed, i.e., with no other free orbital lines than valence lines. (Lines with double arrows represent valence orbitals and those with single arrow valence or non-valence orbitals.) The wave operator is - apart from unity - represented by linked diagrams that are open, i.e., with the final state in the complementary space. All free orbital lines of the wave operator must not be valence lines. (There may also be core lines, not shown, which represent excitations from the closed-shell electron core.)

In the diagrammatic representation the wave operator and the effective Hamiltonian contain diagrams with *closed parts, disconnected from the rest of the diagram*. Such diagrams are said to be *unlinked*, and diagrams free from such parts are *linked*. (It should be observed that with this definition a wave-operator diagram can consist of several disconnected parts and still be linked, if all parts are open.) It can be shown that all unlinked diagram can be made to disappear from the representation of the wave operator and the effective Hamiltonian, provided certain *exclusion-principle-violating diagrams* (EPV) are included. This is the *linked-diagram theorem* (LDT), first demonstrated for closed-shell systems by Brueckner [23] and Goldstone [24] and later extended to the open-shell case with a complete model space by Brandow [25] and others. In the latter case the LDT can be expressed by means of the Bloch eqn (10) as [6, 22]

$$[\Omega, H_0]P = (H'\,\Omega - \Omega H'_{\rm eff})_L P. \tag{19}$$

The second term on the RHS primarily has the effect of eliminating the unlinked diagrams originating from the first term. Some linked parts remain, though, which correspond to the so-called "*folded*" diagrams, first introduced in time-dependent perturbation theory by Morita [26] and later extensively discussed by Kuo et al. [12], Brandow [25] and others. It has been shown by Mukherjee [27, 22] that the LDT can be extended also to *incomplete model spaces*, if the intermediate normalization condition is abandoned. We shall not consider such cases here but restrict ourselves to complete model spaces, spanned by functions of one or several eigenvalues, i.e., to *complete degenerate and quasi-degenerate model spaces*.

3 Time-dependent many-body perturbation theory. Closed-shell case.

The quantum field theory (QFT), as developed in the late 1940's and in the 50's by Feynman, Schwinger, Tomanaga, Dyson and others, is based upon *time-dependent Green's-function* and *time-evolution-operator techniques* [28, 29]. Such techniques have later been extensively used also in non-QFT many-body problems in different fields of physics, particularly for extended systems (see, e.g., [30, 31, 32]). These treatments, however, do not address the particular degeneracy problem, occurring for bound-state systems in atomic/molecular and nuclear physics. Generalization to such systems was done later in the 1960's and 70's, particularly in nuclear physics. In order to be able to merge the QED and MBPT procedures, it will be necessary to rely upon time-dependent techniques. For that reason we shall in the next two sections consider time-dependent many-body theory in the non-relativistic limit, i.e., with *time-independent* perturbations. In section 5 we shall extend the treatment to *time-dependent* interactions and a covariant formulation.

We consider first the case with a single reference state (closed-shell system), which means that the zeroth-order wave functions (ZOF), $\Psi_0 = \Phi$, is known from the start,

$$H_0\Phi = E_0\Phi \quad \text{and} \quad H\Psi = E\Psi. \tag{20}$$

The Hamiltonian is partitioned as before (6), $H = H_0 + H'$. The perturbation H' is *time-independent* but we add an *adiabatic damping factor*

$$H' \rightarrow H'\,\mathrm{e}^{-\gamma|t|}, \tag{21}$$

where γ is a small positive constant, which eventually will go to zero. This has the effect that the perturbation is turned on and off smoothly, so that $H \rightarrow H_0$ and $\Psi \rightarrow \Phi$, when $t \rightarrow \pm\infty$.

We shall work in the *interaction picture*, which means that the operators (O_S) and wave functions ($\Psi_\mathrm{S}(t)$) in the conventional Schrödinger (or Dirac) picture are transformed according to

$$O_\mathrm{I}(t) = \mathrm{e}^{\mathrm{i}H_0 t}\,O_\mathrm{S}\,\mathrm{e}^{-\mathrm{i}H_0 t}; \qquad \Psi_\mathrm{I}(t) = \mathrm{e}^{\mathrm{i}H_0 t}\,\Psi_\mathrm{S}(t). \tag{22}$$

The time-dependent Schrödinger equation then takes the form

$$\mathrm{i}\frac{\partial}{\partial t}\Psi_\mathrm{I}(t) = H'_\mathrm{I}\,\Psi_\mathrm{I}(t), \tag{23}$$

which leads to the implicit formula [28, 30]

$$\Psi_\mathrm{I}(t) = \Psi_\mathrm{I}(t_0) - \mathrm{i}\int_{t_0}^{t}\mathrm{d}t'\,H'_\mathrm{I}(t')\,\Psi_\mathrm{I}(t')$$

or

$$\Psi_\mathrm{I}(t) = U_\gamma(t,t_0)\,\Psi_\mathrm{I}(t_0), \tag{24}$$

where

$$U_\gamma(t,t_0) = 1 + \sum_{n=1}^{\infty}(-\mathrm{i})^n \int_{t_0}^{t}\mathrm{d}t_n \int_{t_0}^{t_n}\mathrm{d}t_{n-1}\ldots\int_{t_0}^{t_2}\mathrm{d}t_1 \times H'_\mathrm{I}(t_n)\,H'_\mathrm{I}(t_{n-1})\ldots H'_\mathrm{I}(t_1)\mathrm{e}^{-\gamma(|t_1|+|t_2|\ldots+|t_n|)}$$

is the (forward) time-evolution operator. It can also be expressed

$$U_\gamma(t,t_0) = 1 + \sum_{n=1}^{\infty} \frac{(-\mathrm{i})^n}{n!} \int_{t_0}^{t} \mathrm{d}t_n \int_{t_0}^{t} \mathrm{d}t_{n-1} \ldots \int_{t_0}^{t} \mathrm{d}t_1 \\ \times T\left[H'_{\mathrm{I}}(t_n)\, H'_{\mathrm{I}}(t_{n-1}) \ldots H'_{\mathrm{I}}(t_1)\right] \mathrm{e}^{-\gamma(|t_1|+|t_2|\ldots+|t_n|)}, \tag{25}$$

where T represents the Wick *time-ordering operator*. (We shall work entirely in the interaction picture in the following and suppress the subscripts I.)

The evolution operator can be represented by means of diagrams in a similar way as operators in time-independent perturbation theory. (As a matter of fact, the diagrammatic representation in MBPT was first developed in this context.)

Gell-Mann and Low [8] have shown that if the limit of

$$|\tilde{\Psi}\rangle = \frac{|\Psi\rangle}{\langle\Phi|\Psi\rangle} = \frac{U_\gamma(0,-\infty)|\Phi\rangle}{\langle\Phi|U_\gamma(0,-\infty)|\Phi\rangle} \tag{26}$$

exists as $\gamma \to 0$, then it represents an exact eigenfunction of the full Hamiltonian [30, p. 61], [28, p. 336],

$$H\frac{|\Psi\rangle}{\langle\Phi|\Psi\rangle} = E\frac{|\Psi\rangle}{\langle\Phi|\Psi\rangle}. \tag{27}$$

The notation $U_\gamma(0,-\infty)$ is a short-hand notation for the limit
$U_\gamma(0,-\infty) = \lim_{t_0\to-\infty} U_\gamma(0,t_0)$. (This limiting process is analysed in detail in several standard texts, e.g., [33, 11]). In addition, the limit $\gamma \to 0$ is always understood.

It should be observed that the numerator and the denominator in (26) become separately singular as $\gamma \to 0$, due to the appearance of *unlinked diagrams*. These are eliminated in the ratio, which therefore remains regular in this limit.

By operating on (27) by $\langle\Phi|$ from the left (and removing the H_0 part), we get the energy shift due to the perturbation

$$\Delta E = E - E_0 = \frac{\langle\Phi|H'|\Psi\rangle}{\langle\Phi|\Psi\rangle} = \frac{\langle\Phi|H'\,U_\gamma(0,-\infty)|\Phi\rangle}{\langle\Phi|U_\gamma(0,-\infty)|\Phi\rangle}. \tag{28}$$

By means of (23) this can also be expressed

$$\Delta E = \mathrm{i}\left[\frac{\partial}{\partial t}\,\ln\langle\Phi|U_\gamma(0,-\infty)|\Phi\rangle\right]_{t=0}. \tag{29}$$

The linked-diagram theorem mentioned above can (for a non-degenerate model space) in the time-dependent formulation be expressed [32]

$$\langle\Phi|U_\gamma(t,t_0)|\Phi\rangle = \exp\langle\Phi|U_\gamma(t,t_0)_{\mathrm{L}}|\Phi\rangle, \tag{30}$$

where the exponent on the rhs contains only *linked diagrams*, as previously defined. Inserted into (29), this yields the important relation

$$\Delta E = \mathrm{i}\left[\frac{\partial}{\partial t}\langle\Phi|U_\gamma(0,-\infty)_{\mathrm{L}}|\Phi\rangle\right]_{t=0}. \tag{31}$$

Since the operator $U_\gamma(t,-\infty)_{\mathrm{L}}$ is regular as $\gamma \to 0$, we can here leave out the subscript γ.

Alternatively, the energy shift can be expressed [28, 30]

$$\Delta E = \mathrm{i}\lambda\gamma \frac{\langle\Phi|\frac{\partial}{\partial\lambda}U_\gamma(0,-\infty)|\Phi\rangle}{\langle\Phi|U_\gamma(0,-\infty)|\Phi\rangle} \tag{32}$$

by introducing a parameter λ in the Hamiltonian, $H = H_0 + \lambda H'$. This formula has been modified by Sucher [9] to

$$\Delta E = \mathrm{i}\frac{1}{2}\lambda\gamma \frac{\langle\Phi|\frac{\partial}{\partial\lambda}U_\gamma(-\infty,-\infty)|\Phi\rangle}{\langle\Phi|U_\gamma(0,-\infty)|\Phi\rangle}, \tag{33}$$

which makes it possible to base the calculation on the *covariant scattering operator* rather than the evolution operator. This is the standard procedure used in bound-state QED calculations. In section 5 we shall develop an alternative procedure by means of the *covariant form of the evolution operator*.

The expression (31) can also be written, again using (23),

$$\Delta E = \langle\Phi|H'\,U_\gamma(0,-\infty)_{\mathrm{L}}|\Phi\rangle. \tag{34}$$

Comparing this with the corresponding (intermediate-normalization) expression in time-independent perturbation theory,

$$\Delta E = \langle\Phi|H'|\Psi\rangle = \langle\Phi|(H'\,\Omega)_{\mathrm{L}}|\Phi\rangle, \tag{35}$$

we see that the wave operator is represented by the *linked, open part* of the evolution operator (also including unity) [28, p. 326], [11, p. 319]

$$\Omega = U(0,-\infty)_{\mathrm{QL}}. \tag{36}$$

In the next section we shall extend this analysis to open-shell systems.

4 Time-dependent many-body perturbation theory. Open-shell case.

The original treatment of Brueckner and Goldstone as well as the Gell-Mann–Low procedure is limited to the case of a single reference state and therefore not directly applicable to general bound-state problems with degenerate (or quasi-degenerate) reference states (open-shell systems). The first attempt to generalize the procedure to the more general case was made by Bloch-Horowitz [34] and Morita [26], but these generalizations were not complete. More complete time-dependent formulations of MBPT were made in the 1970's by several groups [12, 35, 36, 37]. In the present section we shall review this (non-covariant) treatment and in the next section we shall indicate how this can be generalized to a covariant formulation.

In the non-degenerate case (closed-shell system) considered in the previous section, singularities appear in diagrams that are *unlinked*, i.e. with one or several closed parts disconnected from the rest of the diagram. In the degenerate case (open-shell system) singularities may appear also for *connected* diagrams, when a model-space state appears as an intermediate state. Such a diagram is referred to as *reducible*.[1] Irreducible diagrams have no intermediate states in the model space and are *free from singularities*.

[1]Note that we shall later use the concepts reducible and irreducible in a somewhat different sense in connection with the multi-photon interactions; see also Eq. 5.

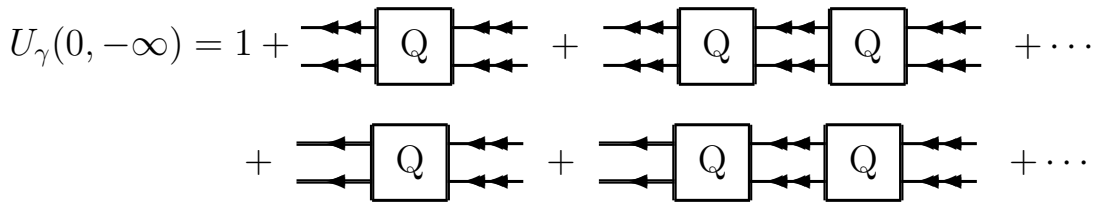


Figure 2: Graphical representation of the evolution operator for open-shell systems. The top row represents the closed part, with the final state in the model space, and the bottom row the open part, with the final state in the complementary space. At least one of the outgoing lines of the open part must be non-valence. The boxes represent irreducible diagram parts with no intermediate states in the model space (Q-box). The states between the Q-boxes lie in the model space. Diagrams with several Q-boxes are reducible.

Generally, a connected evolution-operator diagram can be expressed as a string of irreducible boxes, "*Q-boxes*", separated by states in the model (P) space, as illustrated in Fig. 2 [12]. The irreducible part of the evolution operator is the analogue of the linked part in the non-degenerate case, and we shall denote it by $U_\gamma(0,-\infty)_{\rm L}$. It can be represented by a single (closed or open) Q-box, apart from unity, as depicted in Fig. 3. (For simplicity, we restrict the discussion here to two-body effect, represented by diagrams with two incoming valence lines.) We also introduce

$$U_\gamma(0,-\infty)_{\rm PL}\, P = P\, U_\gamma(0,-\infty)_{\rm L}\, P, \tag{37a}$$

which is the closed part and

$$U_\gamma(0,-\infty)_{\rm QL}\, P = \left[1 + Q\, U_\gamma(0,-\infty)_{\rm L}\right]\, P \tag{37b}$$

the open part of the irreducible evolution operator, including unity.

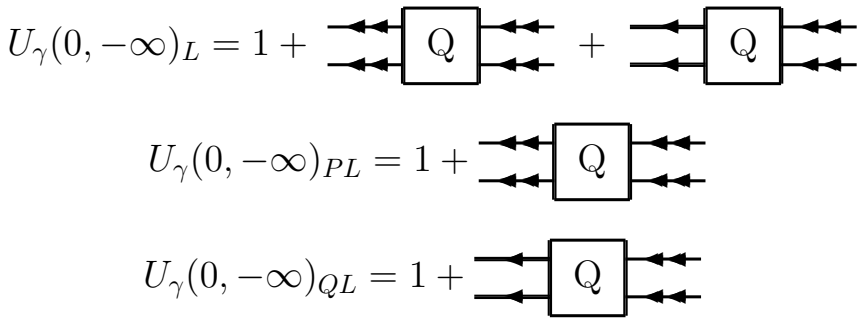


Figure 3: Graphical representation of the irreducible part of the evolution operator (top row) and its closed and open parts. All these parts are free from singularities. (C.f. Fig. 1.) For convenience we include the unity operator also in the open part.

It can be shown that the evolution operator can be *factorized* according to [12, 35, 36]

$$U_\gamma(0,-\infty)|i\rangle = \sum_{j\in D} U_\gamma(0,-\infty)_{\rm QL}\,|j\rangle\,\langle j|\,U_\gamma(0,-\infty)|j\rangle$$

or

$$U_\gamma(0,-\infty)\, P = U_\gamma(0,-\infty)_{\rm QL}\, P\, U_\gamma(0,-\infty)\, P. \tag{38}$$

$U_\gamma(0,-\infty)_{\rm QL}$ is *regular* as $\gamma \to 0$, and *all singularities of the evolution operator are contained in the closed part*, $P\, U_\gamma(0,-\infty)\, P$. This factorization is illustrated in Fig. 4. (Diagram parts

with no free valence lines can be factorized out in a separate way, and we do not consider them further here [12]). It should be noted that in the time-ordered representation we consider in this section, the factorization process also generates "*folded*" diagrams, which compensate for the difference in the time-orderings. These are left out here. Later, in the covariant QED formalism we shall work with Feynman diagrams containing all time-orderings, and folded diagrams of this kind will not appear. Furthermore, it should be noted that the folded diagrams that appear here are of different origin from those appearing in MBPT - although there may be some relation [6].

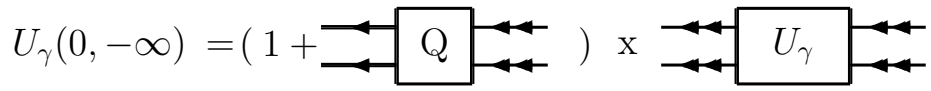


Figure 4: Illustration of the factorization of the evolution operator (38). The smaller box represents the irreducible Q-box and the larger box the closed part of the evolution operator, shown in the top line of Fig. 2.

Kuo et al.[12] have shown that functions $|\phi^\alpha\rangle$, lying in the model space, can be constructed so that

$$|\tilde{\Psi}^\alpha\rangle = \frac{U_\gamma(0,-\infty)|\phi^\alpha\rangle}{\langle\phi^\alpha|U_\gamma(0,-\infty)|\phi^\alpha\rangle} = \frac{U_\gamma(0,-\infty)_{\rm QL}\,P\,U_\gamma(0,-\infty)|\phi^\alpha\rangle}{\langle\phi^\alpha|U_\gamma(0,-\infty)|\phi^\alpha\rangle} \tag{39}$$

are eigenfunctions of the full Hamiltonian, H,

$$H|\tilde{\Psi}^\alpha\rangle = E\,|\tilde{\Psi}^\alpha\rangle \qquad (\alpha = 1,2,\dots d),$$

which is a generalization to degenerate systems of the Gell-Mann–Low relation (26). The eigenvalue equation can be written

$$H\,U_\gamma(0,-\infty)_{\rm QL}\,|\tilde{\Psi}_0^\alpha\rangle = E^\alpha\,U_\gamma(0,-\infty)_{\rm QL}\,|\tilde{\Psi}_0^\alpha\rangle$$

with

$$|\tilde{\Psi}_0^\alpha\rangle = \frac{P\,U_\gamma(0,-\infty)|\phi^\alpha\rangle}{\langle\phi^\alpha|U_\gamma(0,-\infty)|\phi^\alpha\rangle}. \tag{40}$$

By operating on this equation by P from the left, we obtain

$$PHU_\gamma(0,-\infty)_{\rm QL}|\tilde{\Psi}_0^\alpha\rangle = E^\alpha PU_\gamma(0,-\infty)_{\rm QL}|\tilde{\Psi}_0^\alpha\rangle = E^\alpha|\tilde{\Psi}_0^\alpha\rangle, \tag{41}$$

since $PU_\gamma(0,-\infty)_{\rm QL} = P$ according the definition (37b). Equation (41) is of the form of the secular equation (1, 13),

$$H_{\rm eff}|\tilde{\Psi}_0^\alpha\rangle = E^\alpha|\tilde{\Psi}_0^\alpha\rangle.$$

Thus, we have found expressions for the *effective Hamiltonian* in the general (quasi-)degenerate case

$$H_{\rm eff} = PHU_\gamma(0,-\infty)_{\rm QL}P = PH_0P + PH'\,U_\gamma(0,-\infty)_{\rm QL}P. \tag{42a}$$

$$H'_{\rm eff} = PH'\,U_\gamma(0,-\infty)_{\rm QL}\,P. \tag{42b}$$

This is the analogue of the relation (34) in the non-degenerate case. The functions $|\tilde{\Psi}_0^\alpha\rangle$ are the ZOF's, $|\Psi_0{}^\alpha\rangle$. Since $U_\gamma(0,-\infty)_{\rm QL}$ is regular as $\gamma \to 0$, we can leave out the subscript γ. Using (23) we can also express the effective perturbation as [35]

$$H'_{\mathit{eff}} = P\left[\mathrm{i}\frac{\partial}{\partial t}U(t,-\infty)_{\rm PL}\right]_{t=0} P, \tag{43}$$

which is the analogue of (31) in the non-degenerate case. This is a key equation for our procedure. Later we shall indicate that it will be valid also in the covariant treatment of the next section. It should be noted that the effective Hamiltonian (42b) is closed by the perturbation H'. Therefore, it is the closed part of the evolution operator that contributes in the form (43).

By comparing (42a) with the time-independent form of the effective Hamiltonian in intermediate normalization (16b), $H_{\mathit{eff}} = PH\Omega P$, we find in analogy with (36) that the *wave operator* can be identified with the *open, irreducible part* of the evolution operator (including unity)

$$\Omega = U(0, -\infty)_{\mathrm{QL}}. \tag{44}$$

5 Relativistic many-body perturbation theory and QED

5.1 No-virtual-pair approximation

Relativistic many-body perturbation theory (RMBPT) and quantum-electro-dynamics(QED) are tightly connected and have to be considered together. One early primitive starting point for RMBPT was the non-relativistic Hamiltonian (6-8) with the Schrödinger single-electron Hamilton ian replaced by the corresponding Dirac operator

$$H_0 = \sum_{i=1}^{N} h_D(i); \quad h_D = -\boldsymbol{\alpha}\cdot\boldsymbol{p} + \beta m - \frac{\mathrm{e}^2 Z}{4\pi r} + U(r). \tag{45}$$

This suffers from problems due to the appearance of the negative energy states of the Dirac Hamiltonian, the Brown-Ravenhall desease [38]. This can be remedied by introducing *projections operators* [39], which prevent the solutions from falling into the negative *Dirac sea*,

$$H = \Lambda_+ \left[\sum_{i=1}^{N} h_D(i) + \sum_{i<j=1}^{N} \frac{\mathrm{e}^2}{4\pi r_{ij}} - \sum_{i=1}^{N} U(r_i) \right] \Lambda_+. \tag{46}$$

It was first shown by Gaunt that when relativity is taking into account the electron-electron interaction contains in addition to the electrostatic interaction also a *magnetic interaction*, which contributes to the order $(Z\alpha)^2$, where α is the fine-structure constant and Z is the nuclear charge. Shortly afterwards, Breit demonstrated that also the retardation of the interactions contributes to the same order. This leads (in the Coulomb gauge) to the so-called *Breit interaction*

$$B_{12} = -\frac{\mathrm{e}^2}{4\pi} \left(\frac{\boldsymbol{\alpha}_1\cdot\boldsymbol{\alpha}_2}{2r_{12}} + \frac{(\boldsymbol{\alpha}_1\cdot\boldsymbol{r_{12}})(\boldsymbol{\alpha}_2\cdot\boldsymbol{r_{12}})}{2r_{12}^3} \right) \tag{47}$$

and the *projected Coulomb-Breit Hamiltonian*

$$H = \Lambda_+ \left[\sum h_D + \sum \left(\frac{\mathrm{e}^2}{4\pi r_{ij}} + B_{ij} \right) - \sum U(r_i) \right] \Lambda_+. \tag{48}$$

This is the *no-virtual-pair approximation* in the Coulomb gauge (NVPA).

It can be shown by means of QED that the NVPA is in fact quite accurate and *contains all effects of order* $(Z\alpha)^2$ [40, 41]. For light systems this is often sufficient. For heavier systems, for which $Z\alpha$ approaches unity—or when higher accuracy is needed for light systems—it

will be necessary to go beyond this approximation. This can be done by means of QED, as will be demonstrated in the following.

As mentioned in the introduction (5), the multi-photon interaction between the electrons can be separated into *irreducible one-, two-, ... photon interactions*[2] [13],

$$V_{12}^{\text{Irred}} = V_{12}^{(1)} + V_{12}^{(2)} + \dots \tag{49}$$

The Coulomb-Breit interaction (48) is an approximate form of the one-photon interaction, which neglects the effects of retardation and negative-energy states. It will be demonstrated that by means of QED a more complete single-photon interaction can be derived, including these effects. Effects beyond the single-photon interaction are contained in the irreducible multi-photon interactions, and iterating these to self-consistency is, as mentioned, equivalent to solving the *Bethe-Salpeter equation* [14]. In the following we shall indicate how the irreducible multi-photon interactions can be derived.

In addition to the electron-electron interaction there are also other QED effects, such as self-energy interactions and vertex modifications. We shall not be concerned with these effects in the present paper.

5.2 Bound-state QED

The starting point for our QED treatment of bound states will be the time evolution operator (25). In this operator time is evolving only in the *forward* direction. In order to be able to apply the covariant formalism, using Feynman diagrams, we shall generalize this operator by including *forward as well as backward time evolution*.

We consider first the second-order (non-covariant) evolution operator with $t_0 \to -\infty$

$$\begin{aligned} U^{(2)}(t',-\infty) = \frac{(-\mathrm{i})^2}{2} \int_{-\infty}^{t'} \mathrm{d}^4x_2 \int_{-\infty}^{t'} \mathrm{d}^4x_1 \\ \times T\left[\left(-e\psi^\dagger(x)\alpha^\nu A_\nu\psi(x)\right)_2 \left(-e\psi^\dagger(x)\alpha^\mu A_\mu\psi(x)\right)_1\right] \mathrm{e}^{-\gamma(|t_1|+|t_2|)}, \end{aligned} \tag{50}$$

for simplicity leaving out the subscript γ. Here the space integration is over the entire space and the time integration as indicated. We have here introduced the interaction Hamiltonian *density*

$$\mathcal{H}'(x) = -e\psi^\dagger(x)\alpha^\mu A_\mu\psi(x), \quad H_I'(t) = \int \mathrm{d}^3\boldsymbol{x}\, \mathcal{H}'(x) \tag{51}$$

and the *electron-field operators* in the interaction picture

$$\psi(x) = \sum_j \phi_j(x)\, c_j; \quad \psi^\dagger(x) = \sum_j \phi_j^\dagger(x)\, c_j^\dagger. \tag{52}$$

x is the four-dimensional time-space coordinate, $x = x^\mu = (t, \boldsymbol{x})$ [29]. $c_j^\dagger$, c_j are the creation and destruction operators (17), and the four-dimensional single-electron orbitals are $\phi_j(x) = \phi_j(\boldsymbol{x})\, \mathrm{e}^{-\mathrm{i}\varepsilon_j t}$ and $\phi_j^\dagger(x) = \phi_j^\dagger(\boldsymbol{x})\, \mathrm{e}^{\mathrm{i}\varepsilon_j t}$ with $\phi_j(\boldsymbol{x})$ being the eigenfunctions of the Dirac Hamiltonian (45)

$$h_D\, \phi_j(\boldsymbol{x}) = \varepsilon_j\, \phi_j(\boldsymbol{x}). \tag{53}$$

[2]The terms reducible and irreducible interaction should be distinguished from the term reducible and irreducible diagrams, used in the previous section. We refer to an interaction as reducible if there is an intermediate time with no free photons, regardless of the fact whether the intermediate state lies in the model space or in the complementary space.

Generally, an expression like (50) can be evaluated by means of *Wick's theorem*, which states that in second quantization *the time-ordered product is equal to the sum of all possible normal-ordered contractions*, each of which can be represented by a Feynman diagram.

The contraction between electron operators leads to the *electron propagator*, $S_F(x_1, x_2)$, defined by

$$\begin{aligned} \mathrm{i}S_F(x_2,x_1) = \overbrace{\psi(x_2)\,\psi^\dagger(x_1)} = \left\langle 0\left|T\left[\psi(x_2)\,\psi^\dagger(x_1)\right]\right|0\right\rangle = \\ = \left\langle 0\left|\Theta(t_2-t_1)\psi(x_2)\,\psi^\dagger(x_1) - \Theta(t_1-t_2)\,\psi^\dagger(x_1)\psi(x_2)\right|0\right\rangle, \end{aligned} \tag{54a}$$

where $\Theta(t'-t)$ is the Heaviside step function and $\langle 0|$ represents the 'vacuum' state with no particles or holes. With the field operators (52), the electron propagator can be expressed

$$\begin{aligned} \mathrm{i}S_F(x_2,x_1) &= \Theta(t_2-t_1)\,\phi_{j+}(x_2)\,\phi^\dagger_{j+}(x_1) - \Theta(t_1-t_2)\,\phi^\dagger_{j-}(x_1)\,\phi_{j-}(x_2) = \\ &= \Theta(t_2-t_1)\,\phi_{j+}(\boldsymbol{x}_2)\,\phi^\dagger_{j+}(\boldsymbol{x}_1)\,\mathrm{e}^{-\mathrm{i}\varepsilon_j(t_2-t_1)} \\ &\quad -\Theta(t_1-t_2)\,\phi^\dagger_{j-}(\boldsymbol{x}_1)\,\phi_{j-}(\boldsymbol{x}_2)\,\mathrm{e}^{-\mathrm{i}\varepsilon_j(t_2-t_1)}. \end{aligned} \tag{54b}$$

We indicate here by a subscript (+ or -) whether the function represents a particle or a hole state. We employ also the *summation convention* with implicit *summation over repeated indices*.

The electron propagator can be written also as a complex integral, integrated along the real axis,

$$S_F(x_2,x_1) = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi}\, S_F(\boldsymbol{x}_2,\boldsymbol{x}_1,\omega)\,\mathrm{e}^{-\mathrm{i}\omega(t_2-t_1)} \tag{54c}$$

$$S_F(\boldsymbol{x}_2,\boldsymbol{x}_1,\omega) = \frac{\phi_j(\boldsymbol{x}_2)\,\phi^\dagger_j(\boldsymbol{x}_1)}{\omega-\varepsilon_j+\mathrm{i}\eta_j},$$

where j runs over all states and η_j is a small positive quantity with the same sign as ε_j.

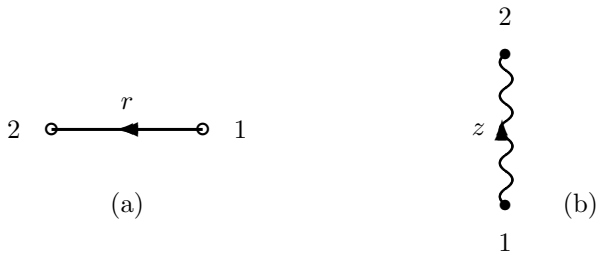


Figure 5: Graphical representation of the electron (a) and photon (b) propagators.

The contraction between the photon operators leads similarly to the *photon propagator*, $D_{F\nu\mu}(x_2 - x_1)$,

$$\mathrm{i}D_{F\nu\mu}(x_2-x_1) = \overbrace{A_\nu(x_2)\,A_\mu(x_1)} = \langle 0|T\left[A_\nu(x_2)\,A_\mu(x_1)\right]|0\rangle, \tag{55a}$$

$$D_{F\nu\mu}(x_2-x_1) = \int \frac{dz}{2\pi}\, D_{F\nu\mu}(\boldsymbol{x}_2-\boldsymbol{x}_1,z)\,\mathrm{e}^{-\mathrm{i}z(t_2-t_1)}.$$

For simplicity we shall work here in the *Feynman gauge*, where

$$D_{F\nu\mu}(\boldsymbol{x}_2-\boldsymbol{x}_1,z) = g_{\nu\mu}\int \frac{\mathrm{d}^3k}{(2\pi)^3}\,\frac{\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{x}_2-\boldsymbol{x}_1)}}{z^2-k^2+\mathrm{i}\eta} = -\frac{g_{\nu\mu}}{2\pi^2\,r_{12}}\int_0^\infty \frac{k\,\mathrm{d}k\,\sin(k\,r_{21})}{z^2-k^2+\mathrm{i}\eta}. \tag{55b}$$

The graphical representations of the propagators are depicted in Fig. 5.

5.3 Single-photon exchange. Covariant form of the evolution operator.

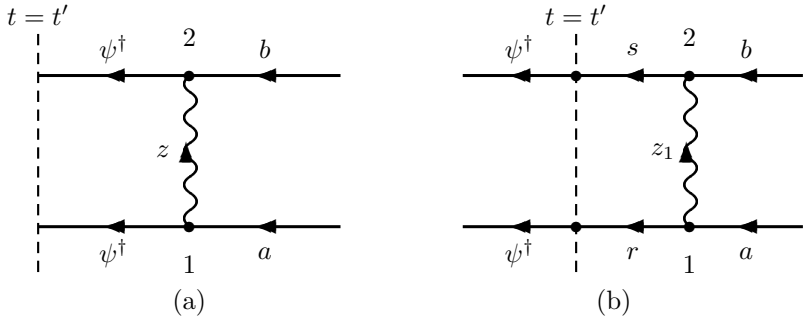


Figure 6: Graphical representation of the evolution operator for single-photon exchange between the electrons.

In order to develop a covariant form of the evolution operator, we consider first the single-photon exchange between the electrons, illustrated in Fig. 6a. Here, there is a contraction between the photon operators but no contraction between the electron operators, and we obtain from (50)

$$U^{(2)}(t',-\infty) = \frac{1}{2}\int_{-\infty}^{t'} \mathrm{d}^4x_2 \int_{-\infty}^{t'} \mathrm{d}^4x_1\, \psi^\dagger(x_2)\,\psi^\dagger(x_1)\, I_{21}\,\psi(x_1)\,\psi(x_2)\,\mathrm{e}^{-\gamma(|t_1|+|t_2|)}, \tag{56}$$

where

$$\begin{aligned} I_{21} &= \mathrm{i}e\alpha_2^\nu\, \mathrm{i}D_{F\nu\mu}(x_2-x_1)\,\mathrm{i}e\alpha_1^\mu; \quad I_{21}(z) = \mathrm{i}e\alpha_2^\nu\, \mathrm{i}D_{F\nu\mu}(\boldsymbol{x}_2-\boldsymbol{x}_1,z)\,\mathrm{i}e\alpha_1^\mu \\ I_{21} &= \int \frac{dz}{2\pi}\, I_{21}(z)\,\mathrm{e}^{-\mathrm{i}z(t_2-t_1)}. \end{aligned} \tag{57}$$

This describes evolution *forward* in time, which corresponds to the situation when $\langle rs|$ are *particle* states. In order to allow also for propagation into *hole* states, integration should also be performed *backwards* in time from $+\infty$ to t' (r and s must here be of the *same sign*). We then make the replacement

$$\int_{-\infty}^{t'} \mathrm{d}t_1 \ldots \Rightarrow \int_{-\infty}^{t'} \mathrm{d}t_2 \ldots + \int_{+\infty}^{t'} \mathrm{d}t_1 \ldots = \int_{-\infty}^{+\infty} \mathrm{d}t_1\, \left[\Theta(t'-t_1)\ldots - \Theta(t_1-t')\ldots\right],$$

which leads to the *covariant form of the evolution operator*

$$\begin{aligned} U^{(2)}_{\mathrm{Cov}}(t',-\infty) &= \frac{1}{2}\iint \mathrm{d}^4x_2\,\mathrm{d}^4x_1\, \Big[\Theta(t'-t_2)\,\psi_+^\dagger(x_2) - \Theta(t_2-t')\,\psi_-^\dagger(x_2)\Big] \\ &\times \Big[\Theta(t'-t_1)\,\psi_+^\dagger(x_1) - \Theta(t_1-t')\,\psi_-^\dagger(x_1)\Big]\, I_{21}\,\psi(x_2)\,\psi(x_1)\,\mathrm{e}^{-\gamma(|t_1|+|t_2|)}. \end{aligned} \tag{58}$$

Here, *the integrations are carried out over all space and time*. The subscripts of the field operators indicate particle and hole part, respectively.

It follows from the definitions used here that

$$\int \mathrm{d}^3\boldsymbol{x}_2\,\psi^\dagger(x_2)\,\mathrm{i}S_F(x_2,x_1) = \Theta(t_2-t_1)\,\psi_+^\dagger(x_1) - \Theta(t_1-t_2)\,\psi_-^\dagger(x_1), \tag{59}$$

which leads to the alternate form of the covariant evolution operator (58)

$$\begin{aligned} U^{(2)}_{\mathrm{Cov}}(t',-\infty) &= \frac{1}{2}\iint \mathrm{d}^3\boldsymbol{x}_2'\,\mathrm{d}^3\boldsymbol{x}_1\,\psi^\dagger(x_2')\,\psi^\dagger(x_1') \\ &\times \iint \mathrm{d}^4x_2\,\mathrm{d}^4x_1\,\mathrm{i}S_F(x_2',x_2)\,\mathrm{i}S_F(x_1',x_1)\, I_{21}\,\psi(x_1)\,\psi(x_2)\,\mathrm{e}^{-\gamma(|t_1|+|t_2|)}, \end{aligned} \tag{60a}$$

using the notations $x_1 = (t_1, \boldsymbol{x}_1)$, $x_1' = (t_1', \boldsymbol{x}_1')$ etc. with $t_1' = t_2' = t'$. By expanding the electron-field operators according to (52) and comparing with the expression (17) for a second-quantized operator, we can identify the matrix elements of the evolution operator,

$$\langle rs|U^{(2)}_{\rm Cov}(t',-\infty)|ab\rangle = \Big\langle rs\Big| \iint \mathrm{d}t_2\,\mathrm{d}t_1\,\mathrm{i}S_F(x_2',x_2)\,\mathrm{i}S_F(x_1',x_1) \times I_{21}\,\mathrm{e}^{it'(\varepsilon_r+\varepsilon_s)}\,\mathrm{e}^{-\mathrm{i}\varepsilon_a t_1-\mathrm{i}\varepsilon_b t_2}\,\mathrm{e}^{-\gamma(|t_1|+|t_2|)}\Big|ab\Big\rangle. \tag{60b}$$

This is represented by the diagram in Fig. 6b. It will be demonstrated later that this covariant form of the evolution operator is equivalent to the *Green's function* used in field theory and can be regarded as the operator form of the two-times Green's function employed by Shabaev and others ([16, 17, 18]).

The standard technique for evaluating expressions like (60b) is to use the integral representation (54c) of the electron propagators and to do the adiabatic switching by means of the time integrals

$$\int_{-\infty}^{\infty} \mathrm{d}t\,\mathrm{e}^{-\mathrm{i}\omega t-\gamma|t|} = \frac{2\gamma}{\omega^2+\gamma^2} = 2\pi\,\Delta_\gamma(\omega); \quad \lim_{\gamma\to 0}\Delta_\gamma(\omega) = \delta(\omega). \tag{61}$$

This leads to rather complicated integrations, and here we shall demonstrate a simpler procedure, by using the time-dependent form of the electron propagator (54b).

The time integral in (58, 60b) is

$$\int_{-\infty}^{\infty}\mathrm{d}t_2\int_{-\infty}^{\infty}\mathrm{d}t_1\,\Big[\Theta(t'-t_2)\,\phi^\dagger_{s_+}(\boldsymbol{x}_2)-\Theta(t_2-t')\,\psi^\dagger_{s_-}(\boldsymbol{x}_2)\Big]\,I_{21}(z) \times\Big[\Theta(t'-t_1)\,\phi^\dagger_{r_+}(\boldsymbol{x}_1)-\Theta(t_1-t')\,\psi^\dagger_{r_-}(\boldsymbol{x}_1)\Big]\,\mathrm{e}^{-\mathrm{i}t_1(q-z)}\,\mathrm{e}^{-\mathrm{i}t_2(q'+z)}\,\mathrm{e}^{-\gamma(|t_1|+|t_2|)},$$

where $q = \varepsilon_a - \varepsilon_r$ and $q' = \varepsilon_b - \varepsilon_s$. Performing the time integrations yields

$$\Big\langle rs\Big||U^{(2)}_{\rm Cov}(t',-\infty)\Big|ab\Big\rangle = = -\Big\langle rs\Big|\int\frac{dz}{2\pi}\,\frac{1}{q-z+\mathrm{i}\gamma_r}\,\frac{1}{q'+z+\mathrm{i}\gamma_s}\,I_{21}(z)\Big|ab\Big\rangle\,\mathrm{e}^{-\mathrm{i}t'(q+q'+\mathrm{i}\gamma_r+\mathrm{i}\gamma_s)}. \tag{62}$$

with $\gamma_r = \gamma\,\mathrm{sgn}(\varepsilon_r)$. We can here identify the denominators as those of the electron propagators (54c) with $\omega = \varepsilon_a - z$ and $\omega = \varepsilon_b + z$, respectively. The advantage of the procedure used here is that we do not have to integrate over the energy parameter of the electron propagators, using the Δ functions (61), but we can directly apply energy conservation at the vertices. Furthermore, in this way we also connect the imaginary part of the electron propagator to the exponent (γ) of the adiabatic damping factor, which we later shall find important in extracting the residual, finite contributions from the singularities (77).

By using the relation

$$\frac{1}{q-z+\mathrm{i}\gamma_r}\,\frac{1}{q'+z+\mathrm{i}\gamma_s} = \left[\frac{1}{q-z+\mathrm{i}\gamma_r}+\frac{1}{q'+z+\mathrm{i}\gamma_s}\right]\,\frac{1}{q+q'+\mathrm{i}\gamma_r+\mathrm{i}\gamma_s},$$

we get after performing the z integration of (62)

$$\Big\langle rs\Big|U^{(2)}_{\rm Cov}(t',-\infty)\Big|ab\Big\rangle = = \Big\langle rs\Big|\int \mathrm{d}k\,f_{21}(k)\left[\frac{1}{q-(k-\mathrm{i}\gamma)\,\mathrm{sgn}(\varepsilon_r)}+\frac{1}{q'-(k-\mathrm{i}\gamma)\,\mathrm{sgn}(\varepsilon_s)}\right]\Big|ab\Big\rangle \times\frac{\mathrm{e}^{-\mathrm{i}t'(q+q'+\mathrm{i}\gamma_r+\mathrm{i}\gamma_s}}{q+q'+\mathrm{i}\gamma_r+\mathrm{i}\gamma_s}, \tag{63}$$

introducing the function

$$f_{21}(k) = -\frac{\mathrm{e}^2 \alpha_1^\mu \, \alpha_{2\mu}}{4\pi^2 \, r_{12}} \, \sin(k \, r_{21}); \quad I_{21}(z) = -\mathrm{i} \int \mathrm{d}k \, \frac{2k \, f_{12}(k)}{z^2 - k^2 + \mathrm{i}\eta}.$$

5.4 Factorization in the covariant formulation

In order to apply the covariant form of the evolution operator to evaluate the effective Hamiltonian and the wave operator for bound-state QED problems it is necessary to generalize the treatment of the previous section. At least for the two-electron systems considered here, it is not difficult to show that the factorization (38) still holds in this formulation with time-dependent interactions, using Feynman graphs. This will be illustrated below with the reducible two-photon ladder interaction. Further details of the factorization will be given in a later publication. From the factorization theorem it follows that also the generalized Gell-Mann–Low formula (39) and the form of the effective Hamiltonian and the wave operator (42a-44) are valid. The main difference from the previous treatment is that the time-dependent interactions will lead to *residual, finite contributions—Model-Space Contributions*—when an intermediate state lies in the model space. This will be discussed further below.

5.5 First-order electron-electron interaction

If the outgoing state $\langle rs|$ lies in the complementary Q space (outside the model space), and since we assumed that r and s have the same sign, then $q + q' \neq 0$, and the expression (63) is regular as $\gamma \to 0$. For $t' = 0$ this is then a contribution to the first-order *wave operator* (44)

$$\Omega^{(1)} = \sum_{|rs\rangle \in Q} \frac{|rs\rangle \langle rs|V(q,q')|ab\rangle}{\varepsilon_a + \varepsilon_b - \varepsilon_r - \varepsilon_s}, \tag{64}$$

where

$$V(q,q') = \int \mathrm{d}k \, f_{21}(k) \left[\frac{1}{q - (k - \mathrm{i}\gamma)\,\mathrm{sgn}(\varepsilon_r)} + \frac{1}{q' - (k - \mathrm{i}\gamma)\,\mathrm{sgn}(\varepsilon_s)} \right] \tag{65}$$

is the *equivalent interaction*.

If the outgoing state $\langle rs|$ lies in the P or model space, then we get a contribution to the first-order *effective Hamiltonian* by means of (43). That this equation is valid also in the covariant formulation, follows from the fact that the relations (23) and (24) still hold. This yields

$$\langle rs|H'_{\mathrm{eff}}|ab\rangle = \langle rs|V(q,q')|ab\rangle. \tag{66}$$

The time derivation eliminates here the singularity occurring for $q + q' = 0$ (and the small denominator that might occur in the quasi-degenerate case). Thus, we see that the first-order wave operator and effective Hamiltonian are given by expressions quite analogous to those of standard time-independent MBPT.

The interaction (65) is the one-photon interaction, mentioned previously (5, 49). The expression *is valid also for elements non-diagonal in energy* and can thus be used in an *iterative process* as well as for evaluating *the effective Hamiltonian of an extended model space*. This should be compared with the standard interaction derived from the S-matrix formalism with energy conservation

$$V_{12}(q) = \mathrm{e}^2 \, \alpha_1^\mu \alpha_2^\nu \, D_{F\nu\mu}(\boldsymbol{x}_2 - \boldsymbol{x}_1, q) = \int \frac{2k \, \mathrm{d}k \, f_{12}(k)}{q^2 - k^2 + \mathrm{i}\eta} = \frac{\mathrm{e}^2 \alpha_1^\mu \alpha_{2\mu}}{4\pi^2 r_{12}} \, \mathrm{e}^{\mathrm{i}|q|r_{12}}, \tag{67}$$

which does not have these properties. It is easy to show that the two expressions (65) and (67) are identical for elements diagonal in energy, i.e., for $q + q' = 0$.

It should be noted that the interaction (65) is *non-hermitian*, which is a consequence of the use of the intermediate normalization (16a), as in ordinary MBPT [6]. By forming the hermitian part of the effective Hamiltonian

$$H_{\rm Herm} = \frac{1}{2}\left(H + H^\dagger\right),$$

the first-order interaction becomes

$$\begin{aligned} V_{\rm Herm}(q,q') &= \frac{1}{2}\left[V_{12}(q,q') + V_{12}(-q,-q')\right] \\ &= \int k\,{\rm d}k\, f_{12}(k)\,\left[\frac{1}{q^2-k^2+{\rm i}\eta} + \frac{1}{q'^2-k^2+{\rm i}\eta}\right], \end{aligned} \tag{68}$$

which is identical to the so-called *Mittleman potential* [15]

$$V_{\rm Mittleman}(q,q') = \frac{1}{2}\left[V_{12}(q) + V_{12}(q')\right].$$

This is also the form of the first-order interaction obtained in the procedure of Shabaev [16, 17, 18]. Numerical calculations show that the differences between the potentials is quite small.

5.6 Relation to Green's functions

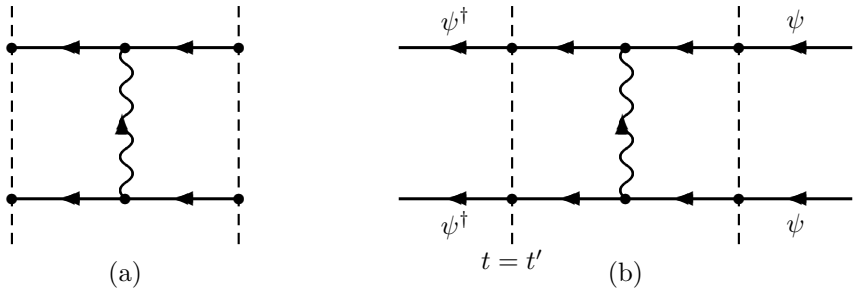


Figure 7: Graphical representation of the Green's function (a) and the evolution operator (b) for single-photon exchange between the electrons. The internal electron lines (between the dots) represent electron propagators and the free lines represent electron-field operators. The dotted lines represent certain times and should not cross any photon line.

The covariant evolution operator employed here is very closely related to the field-theoretical Green's function, frequently used in many-body problems in various field of physics [28, 29, 30] and recently employed in bound-state QED calculations by Shabaev and coworkers [16, 17, 18]. The Green's function corresponding to single-photon exchange, represented graphically in Fig. 7a, can be expressed

$$\begin{aligned} G(x_2', x_1', x_{20}, x_{10}) &= \frac{1}{2}\int {\rm d}^4x_2 \int {\rm d}^4x_1 \\ &\times {\rm i}S_F(x_2', x_2)\,{\rm i}S_F(x_1', x_1)\,I_{21}\,{\rm i}S_F(x_2, x_{20})\,{\rm i}S_F(x_1, x_{10}). \end{aligned} \tag{69}$$

This is a *two-times Green's function*, which implies that there is a single final time, t', and a single initial time, t_0. This we can compare with the corresponding *covariant, two-times*

evolution operator $U^{(2)}_{\rm Cov}(t',t_0)$, which we can get by generalizing the operator (60a),

$$\begin{aligned} U^{(2)}_{\rm Cov}(t',t_0) &= \frac{1}{2}\int \mathrm{d}^3\boldsymbol{x}'_2 \int \mathrm{d}^3\boldsymbol{x}'_1 \int \mathrm{d}^3\boldsymbol{x}_{20} \int \mathrm{d}^3\boldsymbol{x}_{10}\, \psi^\dagger(x'_2)\,\psi^\dagger(x'_1) \\ &\quad \times \int \mathrm{d}^4x_2 \int \mathrm{d}^4x_1\, \mathrm{i}S_F(x'_2,x_2)\,\mathrm{i}S_F(x'_1,x_1)\,I_{21} \\ &\quad \times \mathrm{i}S_F(x_2,x_{20})\,\mathrm{i}S_F(x_1,x_{10})\,\psi(x_{10})\,\psi(x_{20}). \end{aligned} \tag{70}$$

This is illustrated in Fig. 7b. We can then express the evolution operator in terms of the Green's function as

$$\begin{aligned} U^{(2)}_{\rm Cov}(t',t_0) &= \int \mathrm{d}^3\boldsymbol{x}'_2 \int \mathrm{d}^3\boldsymbol{x}'_1 \int \mathrm{d}^3\boldsymbol{x}_{20} \int \mathrm{d}^3\boldsymbol{x}_{10}\, \psi^\dagger(x'_2)\,\psi^\dagger(x'_1) \\ &\quad \times \int \mathrm{d}^4x_2 \int \mathrm{d}^4x_1\, G(x'_2,x'_1,x_{20},x_{10})\,\psi(x_{10})\,\psi(x_{20}). \end{aligned} \tag{71}$$

This relation can be generalized to more complex situations. We see here that the main difference between the two concepts is that the Green's function is a *function*, while the evolution operator is an *operator* with field-operator lines connected to the free vertices. Therefore, *the evolution operator* (70) *can be regarded as the operator form of the two-times Green's function* (69).

5.7 Two-photon electron-electron interaction

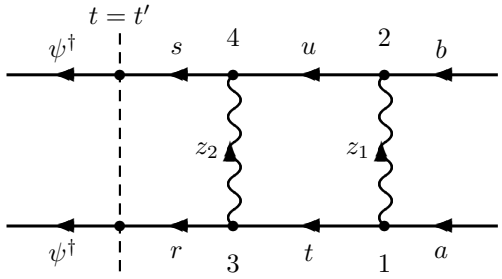


Figure 8: Graphical representation of the evolution operator for the two-photon-photon ladder interaction between the electrons.

We consider next the evolution operator for *the two-photon (ladder) exchange*, illustrated in Fig. 8, and start with the *forward-evolving operator*. Here we make the restrictions in the time-ordering that $t_4 < t_2$ and $t_3 < t_1$, which leaves six possible time-orderings, each of them leading to an equivalent diagram. The time integrations are then

$$\int_{-\infty}^{t'} \mathrm{d}t_4 \int_{-\infty}^{t'} \mathrm{d}t_3 \int_{-\infty}^{t_4} \mathrm{d}t_2 \int_{-\infty}^{t_3} \mathrm{d}t_1.$$

In order to allow for backward evolution into hole states, we perform in analogy with the one-photon case (58-60b). This leads to the covariant evolution operator for the two-photon ladder exchange

$$\begin{aligned} &\left\langle rs \left| U^{(4)}_{\rm Cov}(t',-\infty) \right| ab \right\rangle = \left\langle rs \right| \iint \mathrm{d}^4x_3\,\mathrm{d}^4x_4 \iint \mathrm{d}t_1\,\mathrm{d}t_2 \\ \times\quad & \mathrm{i}S_F(x'_3,x_4)\,\mathrm{i}S_F(x'_3,x_3)\,I_{43}\,\mathrm{i}S_F(x_4,x_2)\,\mathrm{i}S_F(x_3,x_1)\,I_{21} \\ \times\quad & \mathrm{e}^{\mathrm{i}t'(\varepsilon_r+\varepsilon_s)}\,\mathrm{e}^{-\mathrm{i}\varepsilon_a t_1-\mathrm{i}\varepsilon_b t_2}\,\mathrm{e}^{-\gamma(|t_1|+|t_2|+|t_3|+|t_4|)} \Big| ab \Big\rangle. \end{aligned} \tag{72}$$

Performing the time integrations in the same manner as in the single-photon exchange above, leads to

$$\Big\langle rs\,\Big|U^{(4)}_{\rm Cov}(t',-\infty)\Big|\,ab\Big\rangle = \sum_{t,u}\iint \frac{{\rm d}z_1}{2\pi}\,\frac{{\rm d}z_2}{2\pi}\,\frac{1}{(q-z_1-z_2+{\rm i}\gamma_t+{\rm i}\gamma_r)}$$
$$\times\frac{1}{(q'+z_1+z_2+{\rm i}\gamma_u+{\rm i}\gamma_s)}\,\frac{1}{(p-z_1+{\rm i}\gamma_t}\,\frac{1}{(p'+z_1+{\rm i}\gamma_u}$$
$$\times\frac{|rs\rangle\langle rs|2k_2 f_{43}(k_2)|tu\rangle\langle tu|2k_1 f_{21}(k_1)|ab\rangle}{(z_2^2-k_2^2+{\rm i}\eta)(z_1^2-k_1^2+{\rm i}\eta)}\,{\rm e}^{-{\rm i}t'(q+q'+{\rm i}\gamma_r+{\rm i}\gamma_s+{\rm i}\gamma_t+{\rm i}\gamma_u)}. \qquad (73)$$

with $p=\varepsilon_a-\varepsilon_t$; $p'=\varepsilon_b-\varepsilon_u$; $q=\varepsilon_a-\varepsilon_r$; $q'=\varepsilon_b-\varepsilon_s$.

The first denominators in (73) can be rewritten as

$$\frac{1}{(q-z_1-z_2+{\rm i}\gamma_t+{\rm i}\gamma_r)}\,\frac{1}{(q'+z_1+z_2+{\rm i}\gamma_u+{\rm i}\gamma_s)}$$
$$=\left[\frac{1}{(q-z_1-z_2+{\rm i}\gamma_t+{\rm i}\gamma_r)}+\frac{1}{(q'+z_1+z_2+{\rm i}\gamma_u+{\rm i}\gamma_s)}\right]\frac{1}{\Delta E},$$
$$\Delta E = q+q'+{\rm i}\gamma_r+{\rm i}\gamma_s+{\rm i}\gamma_t+{\rm i}\gamma_u,$$

which becomes singular, when the final state lies in the model space. As before, this singularity is eliminated, when the effective Hamiltonian is evaluated according to (43). When the final state lies in the complementary space, we have $q+q'\neq 0$, and the evolution operator gives a contribution to the wave operator (44). When there is no singulartity, the expressions can be evaluated by integrating over z_1 and z_2 as in the S-matrix procedure [42].

5.8 Reducible two-photon ladder interaction

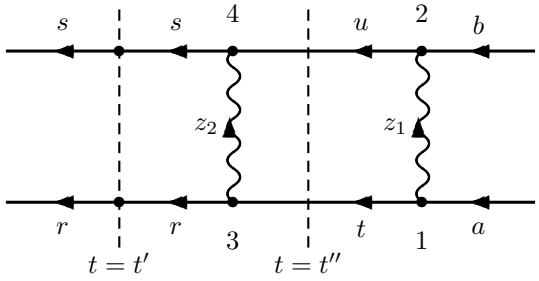


Figure 9: When there is a time between the interactions with no free photons, the two-photon exchange interaction can be separated into two single-photon exchange interactions. This is the "ladder approximation" of the full exchange. This is the reducible part of the interaction, and it contains the singular part of the full two-photon interaction.

A substantial part of the two-photon ladder interaction can be expressed as a ladder of two single-photon interactions of the same type as in standard perturbation theory. Following Bethe and Salpeter and others, we refer to this part as the *reducible* interaction and the remaining part as the *irreducible* interaction (see footnote on p. 12). The reducible two-photon ladder interaction is illustrated in Fig. 9, and for *positive intermediate states* it

can be expressed

$$\begin{aligned}\left\langle rs\left|U^{(4)}_{\rm Cov}(0,-\infty)\right|ab\right\rangle_{\rm Red} &= \\ &= \sum_{t,u}\frac{\langle rs|V_{43}(q+p',q'+p)|tu\rangle\langle tu|V_{21}(q+p',p+p')|ab\rangle}{(q+q')(p+p')} \\ &= \sum_{t,u}\iint {\rm d}k\,{\rm d}k'\,F_{\rm Red}(k,k')\,\langle rs|f_{43}(k')|tu\rangle\,\langle tu|f_{21}(k)|ab\rangle \end{aligned} \tag{74}$$

$$F_{\rm Red}(k,k') = \frac{1}{q+q'}\left[\frac{1}{q+p'-k'}+\frac{1}{q'+p-k'}\right]\frac{1}{p+p'}\left[\frac{1}{p-k'}+\frac{1}{p'-k}\right]$$
$$(p=\varepsilon_a-\varepsilon_t; p'=\varepsilon_b-\varepsilon_u; q=\varepsilon_a-\varepsilon_r; q'=\varepsilon_b-\varepsilon_s)$$

It is easy to show that this has the same singularity as the full ladder interaction, which implies that *the remaining irreducible ladder interaction is non-singular*. The same is true for the *crossed* two-photon interaction, which has no reducible part.

When $\langle tu|$ lies in the model space, the reducible ladder (74) can be expressed

$$\left\langle rs\left|U^{(4)}_{\rm Cov}(0,-\infty)\right|ab\right\rangle_{\rm Red} = \left\langle rs\left|U^{(2)}_{\rm Cov}(0,-\infty\,P\,U^{(2)}_{\rm Cov}(0,-\infty)\right|ab\right\rangle, \tag{75}$$

which is an illustration of the factorization theorem (38) in the covariant formulation. Expanding the denominator of (39) gives rise to *counter terms*, which for $\langle tu| = \langle ab|$ becomes in lowest order

$$-\left\langle rs\left|U^{(2)}\right|ab\right\rangle\left\langle ab\left|U^{(2)}\right|ab\right\rangle = -\frac{\langle rs|V_{43}(q,q')|ab\rangle}{q+q'}\,\frac{\langle ab|V_{21}(0,0)|ab\rangle}{2{\rm i}\gamma}. \tag{76}$$

This cancels exactly the singularity of (74, 75). The situation is similar for the exchange part.

5.9 Model-Space Contribution

As mentioned above, when the interactions are *time-dependent*—as in QED—there will in the factorization process in general be *residual finite contributions* when an intermediate states lies in the model space. We refer to those as the *Model-Space Contribution* (MSC). These contributions can be quite cumbersome to evaluate in the S-matrix formulation, using the Gell-Mann–Low–Sucher procedure. Shabaev has devised an alternative method based on the two-times Green's function, which is free from some of the difficulties in the S-matrix procedure [16], [17], [18]. Here we shall demonstrate a different way of obtaining these contributions, and we take the two-photon electron-electron interaction as an illustration.

In order to study the singularity of (74), we make the substitution $\begin{pmatrix} p\to p+{\rm i}\gamma \\ p'\to p'+{\rm i}\gamma\end{pmatrix}$, which gives

$$\begin{aligned}F_{\rm Red}(k,k') = \frac{1}{q+q'}&\left[\frac{1}{q+p'-k'+{\rm i}\gamma}+\frac{1}{q'+p-k'+{\rm i}\gamma}\right] \\ \times\quad \frac{1}{p+p'+2{\rm i}\gamma}&\left[\frac{1}{p-k+{\rm i}\gamma}+\frac{1}{p'-k+{\rm i}\gamma}\right].\end{aligned} \tag{77}$$

The singularity, which appears for $p + p' = 0$, is of the type

$$D = \frac{1}{\gamma}(A + B\gamma + \dots). \tag{78a}$$

After subtracting the counter term, discussed above, the singular A term vanishes, and to see if there is any *finite contribution* at the singularity, we apply the *l'Hospital rule* (to the entire expression, including the counter term)

$$B = \lim_{\gamma\to 0}\left(\frac{\partial(\gamma D)}{\partial\gamma}\right). \tag{78b}$$

In the present case it can be shown that the counter term does not give any contribution to the finite term. Therefore, the residual, finite contribution—or the *Model-space contribution* (MSC)—of the two-photon exchange (74) is given by

$$MSC_{\rm Red} = \sum_{\varepsilon_t+\varepsilon_u=\varepsilon_a+\varepsilon_b} \iint \mathrm{d}k\,\mathrm{d}k' \lim_{\gamma\to 0}\left[\frac{\partial}{\partial\gamma}(\gamma F_{\rm Red})\right] \langle rs\,|f_{43}(k')|\,tu\rangle\ \langle tu\,|f_{21}(k)|\,ab\rangle\,. \tag{79}$$

It is easy to show that this procedure yields for the two-photon exchange the same result as the conventional procedure [42] but in a much simpler way. It should be noted that the irreducible part of the interaction also have a contribution when the intermediate state is in the model space. Since there is no singularity involved here, we do not here include this in the model-space contribution.

The full two-photon interaction can now be expressed

$$\begin{aligned}\langle rs\,|V_{\rm Two-photon}|\,ab\rangle &= \big\langle rs\,\big|V^{\rm Irred}_{\rm Two-photon}\big|\,ab\big\rangle \\ &+ \sum_{t,u\in Q}\frac{\langle rs\,|V_{43}(q+p',q'+p)|\,tu\rangle\ \langle tu\,|V_{21}(p,p')|\,ab\rangle}{(p+p')} + MSC_{\rm Red}\end{aligned} \tag{80}$$

Here, the first term is the irreducible two-photon ladder and crossed-photon interaction, the second term is the reducible ladder interaction (77) and the last term is the finite contribution (Model-Space Contribution) due to the reducible ladder interaction (79). Note that *intermediate states within the model space are excluded from the reducible part but are included in the (regular) irreducible part.* Note that the states t and u must either both be particle states or both hole states. The contribution where the states are of different kind is included in the irreducible part.

5.10 The Bethe-Salpeter equation

The procedure described above for the two-photon interaction can in principle be generalized to arbitrary multi-photon interactions. We can separate out the *irreducible* one-, two-, three- ... photon interactions

$$V^{\rm Irred}_{21} = V^{(1)}_{21} + V^{(2)}_{21} + V^{(3)}_{21} + \dots, \tag{81}$$

and the complete electron-electron interaction is essentially reproduced by iterating these to all orders. This can be represented as a Green's-function equation

$$\begin{aligned}G(x_2',x_1',x_{20},x_{10}) &= \mathrm{i}S_F(x_2',x_{20})\,\mathrm{i}S_F(x_1',x_{10}) \\ &+ \int \mathrm{d}^4x_2 \int \mathrm{d}^4x_1\,\overline{K}(x_2',x_1',x_2,x_1)\,G(x_2,x_1,x_{20},x_{10}) + MSC_{\rm Red}\end{aligned} \tag{82}$$

where $\overline{K}$ represents the irreducible *kernel* and $MSC_{\rm Red}$ is the model-space contribution of the reducible part. This corresponds to the *complete Bethe-Salpeter equation* for the electron-electron interaction, illustrated graphically in Fig. 10 [14, 30]. The model-space is excluded from the intermediate states between the irreducible parts, which makes the expression regular.

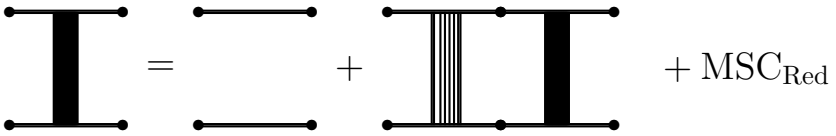


Figure 10: Graphical representation of the complete Bethe-Salpeter equation in the form of a Dyson equation. The solid area represents the two-particle propagator or Green's function and the dashed area the irreducible kernel. The MSC represents the model-space contribution of the reducible part.

It follows from what is said above that the irreducible multi-photon interactions can be handled very much like the interactions in standard MBPT. *The irreducible interactions are free from singularities.* The intermediate states between the interactions are restricted to the Q space, as in ordinary MBPT, while inside the interactions *all* intermediate states (Q as well as P space) should be included. In addition, there will be finite model-space contributions (MSC) of the reducible part, which can be obtained by means of the l'Hospital rule, as described above.

The procedure outlined here is presently being investigated further, and more details together with numerical illustrations, will be published in a forthcoming paper [19].

6 Summary and outlook

The conventional procedure for atomic QED calculations on bound systems is based upon the S- matrix formalism and the adiabatic damping procedure of Gell-Mann–Low and Sucher. This procedure has certain shortcomings and cannot be used to construct a secular equation with an effective Hamiltonian for general open-shell systems. In this paper a procedure is described for constructing such an effective Hamiltonian, applicable also to a model space with degenerate or quasi-degenerate unperturbed energy levels (*extended model space*). The effective Hamiltonian constructed in this way is free from singularities. It is also shown that the electron-electron interaction can be separated into non-singular *irreducible one-, two-, ... photon interactions.* In principle, these can be iterated as in standard MBPT. Including all multi-photon interactions to all orders is equivalent to solving the *Bethe-Salpeter equation.* Singularities do not appear, but intermediate states in the model space give rise to finite contributions, which can be evaluated by a limiting process.

We have here concentrated on the photon exchange between the electrons. In principle also other radiative effects could be included in the procedure. The vertex modifications can be included in the irreducible multi-photon interactions. The vacuum polarization can be treated as a potential perturbation, generating new single-electron states. The electron and photon self-energy interactions can be treated by modifying the electron and photon propagators. In this way it seems possible - at least in principle - to merge QED and MBPT together in a rigorous and systematic way. The irreducible multi-photon interactions obtained in this process can be iterated in very much the same way as in ordinary MBPT. Since these interactions can at present only be obtained in a numerical way, it may not be feasible to use them, beyond the simplest ones, in practical calculations on more complex

structures. The procedure may be used, though, to test various approximations, and the more complete scheme described here can then be used for benchmarking.

Acknowledgements

It is a great pleasure for me to contribute to this volume in honour of Charlotte Froese-Fischer. Charlotte has played a world-leading role in the field of atomic-many-body theory for more than three decades. Many generations of new scientists have been educated in the field of atomic structure, which has improved the level of scientific works both in experiments and theory.

The author also wishes to acknowledge stimulating collaboration and discussions with Thomas Beier, Martin Gustavsson, Paul Indelicato, Eva Lindroth, Ann-Marie Mårtensson-Pendrill, Hans Persson, Sten Salomonson, Vladimir Shabaev, Per Sunnergren, and Björn Åsen. This work has been supported in part by an award from the Alexander von Humboldt Foundation.

References

[1] Hermanspahn N., Häffner H., Kluge H.-J., Quint W., Stahl S, Verdu J., and Werth G., *Phys. Rev. Lett.* Jan 2000 and private communication

[2] Persson H., Salomonson S., Sunnergren P., and Lindgren I., *Phys. Rev.* A**56**, R2499 (1997)

[3] Beier T., Lindgren I., Persson H., Salomonson S., and Sunnergren P. (accepted for publication in *Phys. Rev.*)

[4] Mooney T., Lindroth E., Indelicato P., Kessler Jr. E.G., and Deslattes R.D., *Phys. Rev.* A**45**, 1531 (1992); Kessler E.G., Deslattes R.D., Girard D., Schwitz W., Jacobs L., and Renner O., *Phys. Rev.* A**26**, 2696 (1982)

[5] Indelicato P., and Lindroth E., *Phys. Rev.* A**46**, 2426 (1992); Indelicato P., Boucard S., and Lindroth E., *Eur. Phys.* J. D**3**, 29 (1998).

[6] Lindgren I. and Morrison J., *Atomic Many-Body Theory*, Sec. ed., Springer Verlag (1986)

[7] Møller, *Klg Danske Vidensk. Selsk. Mat.-Fys. Medd.* **23**, No 1 (1945)

[8] Gell-Mann M., and Low F., *Phys. Rev.* **84**, 150 (1951)

[9] Sucher J., *Phys. Rev.* **107**, 1448 (1957)

[10] Mårtensson-Pendrill A.-M., Lindgren I., Lindroth E., Salomonson S., and Staudte D.S., *Phys. Rev.* A**51**, 3630 (1995)

[11] Roman P., *Advanced Quantum Theory*, Addison-Wesley Publ. co. (1965)

[12] Kuo T.T.S., Lee S.Y., and Ratcliff K.F., *Nucl. Phys.* A**176**, 65 (1971)

[13] Lindgren I., *Nucl. Instr. Meth.* B**31**, 102 (1988); Lindgren I., in *Program on Relativistic Quantum Electrodynamics and Weak Interaction Effects in Atoms*, Institute of Theortical Physics, Santa Barbara, Jan-June 1988, AIP Conf. Series **189**, p. 371

[14] Bethe H.A. and Salpeter E.E., *Phys. Rev.* **82**, 309 (1951), *ibid.* 84, 1232 (1951); *Quantum Mechanics of One- and Two-Electron Atoms*, Springer-Verlag (1957)

[15] Mittleman M.H., *Phys. Rev.* A**5**, 2395 (1972)

[16] Shabaev V.M. and Fokeeva I.G., *Phys. Rev.* A**49**, 4489 (1994)

[17] Shabaev V.M., *Sov. Phys. J.* **33**, 660 (1990); *J. Phys.* A**24**, 5665 (1991); *J. Phys.* B**26**, 4703 (1993); *Phys. Rev.* A**50**, 4521 (1994)

[18] Yerokhin V.A., Artemyev A.N., Beier T., Plunien G., Shabaev V.M., and Soff G., *Phys. Rev.* A**60**, 3522 (1999)

[19] Lindgren I., Salomonson S., and Åsén B., (in preparation)

[20] Bloch C., *Nucl. Phys.* **6**, 329 (1958, *ibid.* **7**, 451 (1958)

[21] Lindgren I., *J. Phys.* B**7**, 2441 (1974)

[22] Lindgren I. and Mukherjee D.,*Phys. Rep.* **151**, 93 (1987)

[23] Brueckner K.A., *Phys. Rev.* **100**, 36 (1955)

[24] Goldstone J., *Proc. Roy. Soc.* A**239**, 267 (1957)

[25] Brandow B.H., *Rev. Mod. Phys.* **39**, 771 (1967)

[26] Morita T., *Prog. Theor. Phys.* **29**, 351 (1963)

[27] Mukherjee D., *Chem. Phys. Lett.* **125**, 207 (1986)

[28] Schweber S.S., *An Introduction to Relativistic Quantum Field Theory*, Row, Peterson and Co. (1961)

[29] Itzykson C. and Zuber J.-B., *Quantum Field Theory*, McGraw-Hill (1980)

[30] Fetter A.L., and Walecka, J.D., *Quantum Theory of Many-Particle Systems*, McGraw-Hill (1971)

[31] Thouless D.J., *The Quantum Mechanics of Many-Body Systems*, Acad. Press (1972)

[32] March N.H., Young W.H., and Sampanthar S., *The Many-Body Problem in Quantum Mechanics*, Cambridge Univ. Press (1967)

[33] Nozieres P., *The Theory of Interacting Fermion Systems*, Benjamin (1965)

[34] Bloch C. and Horowitz J., *Nucl. Phys.* **8**, 91 (1958)

[35] Jones R.W. and Mohling F., Nucl. Phys. A **151**, 420 (1970)

[36] Oberlechner G., Owono-N'-Guema F., and Richert J., *Nouvo Cimento* B**68**, 23 (1970)

[37] Johnson M. and Baranger M., *Ann. of Phys.* (N.Y.) **62**, 172 (1971)

[38] Brown G.E. and Ravenhall D.G., *Proc. Roy. Soc.* London A**208**, 552 (1951)

[39] Sucher J., *Phys. Rev.* A**22**, 348 (1980)

[40] Sucher J., *J. Phys.* B**21**, L585 (1988)

[41] Lindgren I., *J. Phys.* B**23**, 1085 (1990)

[42] Lindgren I., Persson H., Salomonson S., and Labzowsky L., *Phys. Rev.* A**51**, 1167 (1995)