Einstein Centennial Review Paper: Many-body-QED perturbation theory: Connection to the two-electron Bethe-Salpeter equation

Ingvar Lindgren, Sten Salomonson, and Daniel Hedendahl

Abstract: The connection between many-body perturbation theory (MBPT) and quantum-electrodynamics (QED) is reviewed for systems of two fermions in an external field. The treatment is mainly based upon the recently developed covariant-evolution-operator method for QED calculations [Lindgren *et al.* Phys. Rep. **389**, 161 (2004)], which has a structure quite akin to that of MBPT. At the same time this procedure is closely connected to the S-matrix and the Green's-function formalisms and can therefore serve as a bridge between various approaches. It is demonstrated that the MBPT-QED scheme, when carried to all orders, leads to a Schrödinger-like equation, equivalent to the Bethe-Salpeter (BS) equation. A Bloch equation in commutator form that can be used for an "extended" or quasi-degenerate model space is derived. This is a multi-state equation that has the same relation to the single-state BS equation as has the standard Bloch equation to the ordinary Schrödinger equation. It can be used to generate a perturbation expansion compatible with the BS equation also for a quasi-degenerate model space.

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1. Introduction

1.1. General

What is known as the Bethe-Salpeter (BS) equation represents the complete solution of the relativistic two-body problem with important applications in various branches of physics. The equation was first derived by Bethe and Salpeter in 1951 [1], using the relativistic S-matrix formalism and the analogy with Feynman graphs, and at about the same time by Gell-Mann and Low [2], using a rigorous field-theoretical approach based on Green's functions. A closely related equation was discussed by Schwinger in his Harvard lectures already in the late 1940's [3, 4, 5, 6].

In interpreting the solutions of the BS equation, several serious problems were encountered, as discussed early by Dyson [7], Wick [8] and Goldstein [9]. Dyson was particularly concerned about the meaning of the wave function in relativistic quantum mechanics, a subject *"full of obscurities and unsolved problems"*. Solving the BS equation leads to a wave function with individual times for the two particles. This function is manifestly relativistically covariant but not in accordance with the

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standard quantum-mechanical picture. That leads to ”spurious” or ”abnormal” solutions without physical significance and with no nonrelativistic counterpart [10]. Another fundamental problem is that the BS equation does not reduce to the correct ”one-body limit”, when one of the particles becomes infinitely heavy, as discussed by Gross and others [11, 12]. Problems of these kinds are most pronounced in the scattering of strongly interacting particles but less so for bound-state systems in weak-coupling [13, 14, 15, 16, 17] (see ref. [6] for a review).

The earliest applications of the BS equation appeared in atomic physics and concerned the proton recoil contribution to the hydrogen fine structure by Salpeter [18] and the positronium energy level structure by Karplus and Klein [4].

An important goal for the equation has been the study of *strongly interacting particles*, which is a fundamental problem in elementary-particle physics. In recent years there have been numerous applications in QCD, dealing mainly with the quark-quark, quark-antiquark interactions, quark confinement and related problems [14, 19, 20, 21]. Here, the problems mentioned above are more serious, as recently summarized by Namyslowski [6].

There have also been many applications in surface and solid-state physics, ranging from electron-hole interactions in ion crystals [22] and studies of the two-dimensional Hubbard model [23] and Cooper pairs [24] to quantum dots [25].

The BS equation has also been applied to three or more particles [26, 27, 28], although serious problems have been encountered for more than three particles [29].

Various approximation schemes for treating the BS equation have been developed over the time. The simplest approximation is the *”ladder approximation”*, where all intermediate states evolve only in the forward (positive) time direction. This is a useful starting point in the strong-coupling case, where the standard perturbative or self-consistent approach may not converge, and this approximation is, for instance, the basis for the Brueckner theory of nuclear matter [30, 31, Sect. 41]. Another approach is the *”quasi-potential approximation”*, which implies that the equation is reduced to an equivalent 3-dimensional Schrödinger equation, which can be done without loosing any rigor [14, 32]. Early numerical calculations in this regime were done particularly by Schwartz and Zemach [33] and Kaufmann [34].

In atomic physics the BS equation has been applied mainly in treating positronium [35, 36] and heliumlike ions, and we shall be particularly concerned here with the latter. This is strictly speaking a three-body problem but can to a good approximation be treated—with the first Born approximation—as a two-body problem with an external potential. The application to heliumlike systems was pioneered by Sucher [37, 38] and Araki [39] in the late 1950’s for deriving the leading relativistic and QED energy corrections beyond the Breit interaction. Later these works have been extended—largely along the lines of Sucher—by Douglas and Kroll in the 1970’s [40] and more recently by Zhang and Drake [41, 42, 43, 44].

The technique developed by Drake and coworkers is presently the most accurate available one in dealing with heliumlike systems. The wave functions used are very accurate functions of Hylleraas type, and the QED corrections are evaluated by means of analytical expressions up to order α^5 Ry (atomic units, or $m\alpha^7$ in relativistic units), derived from the BS equation. The wave functions used by Drake et al. are nonrelativistic but certain relativistic effects are treated to all orders in the ”*unified model*” [45, 46]. The analysis of the BS equation are in these works based upon the *Brillouin-Wigner perturbation theory* (BWPT).

A different and in some aspects more versatile approach to the many-body problem is the procedure known as the *many-body perturbation theory* (MBPT). This is based upon *Rayleigh-Schrödinger perturbation theory* (RSPT) [47], which via the Bloch equation can be used to derive various computational schemes, such as the *linked-diagram expansion* (LDE) [48, 49, 50]. A particularly powerful technique is the *Coupled-Cluster Approach* (CCA) [51, 52, 53], which is widely used in quantum chemistry [54, 55]. This technique is strictly speaking non-perturbative but can also be regarded as an ”*all-*

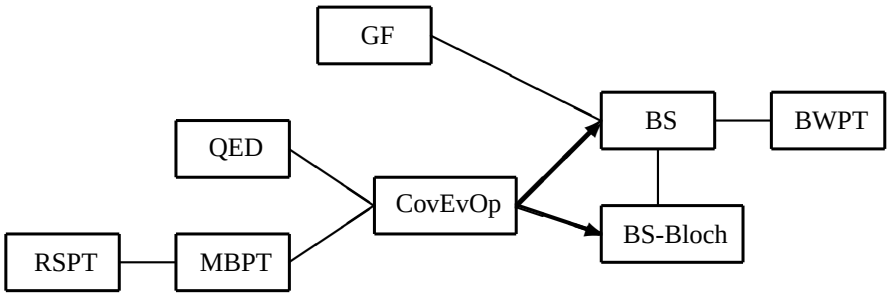


Fig. 1. Schematic illustration of the connection between various many-body techniques. The upper right part represents the Green's-function (GF) approach, which is used to derive the Bethe-Salpeter (BS) equation, normally analyzed in terms of the Brillouin Wigner perturbation theory (BWPT). The lower-left part illustrates the many-body perturbation theory (MBPT), originating from Rayleigh-Schrödinger perturbation theory (RSPT). The combination of quantum-electrodynamics (QED) with MBPT is represented by the covariant-evolution-operator (CovEvOp) method, and the link to the BS equation and the corresponding Bloch equation—the main subject of the present paper—is illustrated by the arrows.

order" perturbative expansion, and we shall include it in the MBPT category here. The MBPT techniques are primarily developed for the weak-coupling case, but might in the non-perturbative (CCA) form be used also in strong coupling.

The MBPT procedures, based initially upon RSPT, have the great advantage compared to techniques based upon BWPT that they are *size-extensive* in each order, which implies that the energy scales linearly with the size of the system—a property of vital importance for molecular problems [56, 57]. The MBPT procedures can also be combined with the *extended-model-space technique*, which is particularly effective in dealing with problems of *quasi-degeneracy* [58, 59, 47, 60].

For QED problems the S*-matrix technique* has been the standard procedure since the days of Feynman and Dyson. (For a review of the application to bound-state problems, see ref. [61].) Being based upon scattering theory, this technique has the disadvantage that its structure is quite different from that of MBPT, which makes it hard to combine the procedures (see, e.g. ref. [62]). The standard procedure for such a combination has been to perform a separate (relativistic) many-body calculation and adding first-order energy corrections from QED analytically [63]. This procedure gives in many cases satisfactory results but is hard to improve in any systematic way. In particular, it gives no additional information about the wave function.

Another disadvantage with the S-matrix formalism is that the energy is conserved between the initial and the final states. This implies that it cannot be combined with the extended-model-space technique, successfully applied in MBPT. This technique requires generally elements of the effective interaction that are nondiagonal in energy. This problem has recently been remedied by means of a new technique, known as the *Covariant-Evolution-Operator method* (CovEvOp), which is a modification of the standard evolution-operator technique of time-dependent perturbation theory [31] in order to make it applicable to relativistic problems (for a review, see ref. [64]). This technique has a structure that is very akin to that of MBPT, and it deals with the key ingredients of MBPT—the wave operator and the effective interaction. At the same time the method is closely related to the S-matrix formalism and the Green's-function procedure. The technique can therefore be regarded as a merger of MBPT/CCA and QED [65], and it has recently been successfully applied to the quasi-degenerate fine-structure states of heliumlike systems [66].

The quasi-degenerate problem can also be handled with the *two-time Green's-function* approach, developed by Shabaev and coworkers (for a review, see ref. [67]). This technique, however, has no direct link to MBPT and will therefore not be discussed further here.

The procedure with the Covariant-Evolution-Operator method is now being further developed at our laboratory in order to combine QED and MBPT in a more complete fashion. This will be based on the relativistic coupled-cluster approach (CCA) of electron correlation or the so-called Dirac-Coulomb approximation, corresponding to the (all-order) "ladder approximation" of the Bethe-Salpeter equation. This is combined with a perturbative (order-by-order) expansion of the remaining (mainly QED) effects, which in principle leads to the full BS equation. This is along the lines early drawn by Sucher [38] and followed by many later works [40, 15, 43, 36, 68]. Our approach differs from all the earlier ones in the sense that all effects are evaluated *numerically* rather than analytically.

Our approach implies that the QED effects are evaluated with highly correlated (relativistic) wave functions, and for two-electron systems the results will then, in principle, be comparable to those of Drake's unified method, with the difference that the relativistic effects are included in a complete way and that the QED effects are evaluated numerically.

In the diagram in Fig. 1 we have tried to represent the relations between the many-body approaches described here in a simple and illustrative way. The many-body procedures based upon Rayleigh-Schrödinger perturbation theory are indicated in the lower-left part and the Green's-function and Bethe-Salpeter procedures, more associated to Brillouin-Wigner perturbation theory, in the upper-right part. The present paper deals particularly with the connection between the two approaches, represented by the arrows in the diagram.

In addition to deeper insight into the different procedures, the present treatment will make it possible to analyze a problem based on the BS equation in terms of RS-MBPT—not only in terms of BWPT, as has previously been the case [40, 44]. The corresponding Bloch equation in commutator form, which we have derived, has the same relation to the BS equation as has the standard Bloch equation to the ordinary Schrödinger equation, and it could possibly be used to eliminate the quasi-degeneracy problem that might appear when the BS equation is treated for a single state at a time.

Since the equivalence of the MBPT-QED-CovEvOp procedure with the BS equation has now been established for two-electron systems, this new link will probably make it easier to apply the BS procedure—or its equivalence— also to systems with more electrons. Alternatively, this can be used to analyze a many-body-QED calculation to find out what is missing in order to represent a complete Bethe-Salpeter treatment. Our main emphasis here is on applications to atoms and other weakly interacting systems. Since the procedure we have developed, however, is based upon a combination of perturbative and non-perturbative approaches, the results obtained might be useful also outside this regime.

The paper will be organized in the following way. Below we shall first conjecture the Bethe-Salpeter equation in a simple-minded way as an introduction. In section 2 we shall summarize the necessary ingredients of time-independent and time-dependent perturbation theory and in the following section briefly review the original derivations of the Bethe-Salpeter equation by Bethe and Salpeter and by Gell-Mann and Low, based on Green's functions. The main part of the paper will be devoted to a rigorous derivation of the Bethe-Salpeter equation, starting from the covariant-evolution-operator method. The basics of the method are summarized in section 4, and the method will in the following section be used to derive the Bethe-Salpeter equation. A corresponding Bloch equation will also be derived, which will make it possible to treat the BS equation perturbatively or iteratively also for a quasi-degenerate (extended) model space. Technical details of the treatment are given in a number of appendices. Radiative effects (self energies and vacuum polarization) are not considered here but can be included by modifying the electron propagator and photon interactions, as discussed, for instance, by Douglas and Kroll [40].

1.2. Bethe-Salpeter equation

An equation of BS type can be conjectured in a very simple way by considering the time-independent nonrelativistic Schrödinger equation

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

with $H = H_0+V_1$, where $H_0 = h_1+h_2$ is the zeroth-order Hamiltonian (sum of single-electron Hamiltonians) and $V_1 = e^2/r_{12}$ is the electron-electron interaction (in relativistic units [1]). The Schrödinger equation can then be expressed

$$(E - H_0)|\Psi\rangle = V_1|\Psi\rangle \tag{2}$$

with the solution

$$|\Psi\rangle = \Gamma(E)V_1|\Psi\rangle \tag{3}$$

where

$$\Gamma(E) = \frac{1}{E - H_0} = \frac{|rs\rangle\langle rs|}{E - \varepsilon_r - \varepsilon_s} \tag{4}$$

is the *"resolvent"* operator [47, Ch. 9] and $|rs\rangle$ is the Dirac notation of the straight (not antisymmetrized) product of two single-electron functions, satisfying the Dirac equation

$$h|i\rangle = \varepsilon_i|i\rangle \tag{5}$$

We apply the summation convention, implying summation over repeated indices appearing on one side of the equation. Unless specified otherwise, the summation is performed over positive- (particle) as well as negative-energy (hole) states.

In the relativistic formalism one should, following Sucher [37, 38], replace V_1 by $\Lambda_{++}e^2/r_{12}\Lambda_{++}$, where Λ_{++} is the projection operator for particle (positive-energy) states. This leads to the *Coulomb-ladder approximation*, mentioned above, i.e., a series of Coulomb interactions separated by particle states. In QED, V_1 can in the first approximation be replaced by the *energy-dependent* interaction with a fully *covariant photon* $V_1(E)$, accounting for the instantaneous Coulomb interaction and the (retarded) Breit interaction. In the next step $V_1(E)$ can be replaced by $V_1(E) + V_2(E)$, where $V_2(E)$ represents the *non-separable* (irreducible) interaction of two photons, i.e., the interaction of two covariant photons that in the QED description cannot be represented by repeated single-photon interactions (see Fig. 6 below). Continuing this process, summing all non-separable interactions with one, two, ... photons

$$\mathcal{V}(E) = V_1(E) + V_2(E) + \cdots \tag{6}$$

leads to

$$|\Psi\rangle = \Gamma(E)\,\mathcal{V}(E)|\Psi\rangle \tag{7}$$

or

$$(E - H_0)\,|\Psi\rangle = \mathcal{V}(E)|\Psi\rangle \tag{8}$$

This is equivalent to the Schrödinger-like form of the *Bethe-Salpeter equation* derived by Sucher [38, Eq. 1.47] and also used by Douglas and Kroll [40, 3.26] and by Zhang [43, Eq. 15].

The BS equation (8) can be expanded in terms of a Brillouin-Wigner perturbation series [47, Ch. 9]

$$|\Psi\rangle = |\Psi_0\rangle + \Big(\Gamma_Q(E)\,\mathcal{V}(E) + \Gamma_Q(E)\,\mathcal{V}(E)\Gamma_Q(E)\,\mathcal{V}(E) + \cdots\Big)\big|\Psi_0\big\rangle \tag{9}$$

where Ψ_0 is the unperturbed wave function and

$$\Gamma_Q(E) = \frac{Q}{E - H_0} \tag{10}$$

[1] In this article relativistic units are used, i.e., $m = c = \hbar = \epsilon_0 = 1, e^2 = 4\pi\alpha$, where α is the fine-structure constant.

is the "reduced" resolvent (4) with the unperturbed state removed. For this sequence to converge properly, it is required that there be no eigenstate of H_0 close in energy to that of Ψ_0 and of the same symmetry. A rigorous derivation of the equation will be given in the following sections.

2. Conventional many-body perturbation theory

2.1. Time-independent perturbation theory

In time-independent many-body perturbation theory (MBPT) (see, e.g., ref. [47]) the aim is to solve the Schrödinger equation by successive approximations for a number of *"target"* states

$$H\,|\Psi^\alpha\rangle = E^\alpha\,|\Psi^\alpha\rangle\,; \qquad (\alpha = 1, 2, \cdots d) \tag{11}$$

($\boldsymbol{x}$ stands here for all space coordinates, leaving out spin coordinates). The time-independent Hamiltonian is partitioned into a zeroth-order Hamiltonian and a perturbation

$$H = H_0 + H' \tag{12}$$

For each target state $|\Psi^\alpha\rangle$ there exists a *model state* $|\Psi_0^\alpha\rangle$ (corresponding to the *"zeroth-order wave function"*, ZOWF) that is confined to a subspace, the *model space* (P), spanned by eigenstates of H_0. The model space can be degenerate or non-degenerate (quasi-degenerate). In the latter case the model states are not necessarily eigenstates of H_0. It is always assumed that all degenerate states of H_0 are either entirely inside or entirely outside the model space.

A *wave operator* Ω can be defined so that it transfers all model states to the corresponding target states

$$\boxed{|\Psi^\alpha\rangle = \Omega\,|\Psi_0^\alpha\rangle\,; \qquad (\alpha = 1, 2, \cdots d)} \tag{13}$$

In the following we shall use the *intermediate normalization* (IN), implying that

$$\big\langle \Psi_0^\alpha \big| \Psi^\alpha \big\rangle = 1 \tag{14}$$

The model states are the projections of the target states on the model space

$$|\Psi_0^\alpha\rangle = P|\Psi^\alpha\rangle \tag{15}$$

which implies

$$P\Omega P = P \tag{16}$$

The exact energies as well as the model states are obtained by solving the secular equation

$$H_{\rm eff}\,|\Psi_0^\alpha\rangle = E^\alpha\,|\Psi_0^\alpha\rangle, \tag{17}$$

within the model space. Here, $H_{\rm eff}$ is the *effective Hamiltonian*, in IN given by

$$H_{\rm eff} = PH\Omega P \tag{18}$$

The wave operator satisfies the *generalized Bloch equation* [58, 47]

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

where $H'_{\rm eff}$ is the *effective interaction* (in IN)

$$H'_{\rm eff} = H_{\rm eff} - PH_0P = PH'\Omega P \tag{19b}$$

For a degenerate model space with the energy E_0 the equation goes over into the original Bloch equation [69, 70]

$$(E_0 - H_0)\,\Omega P = \big(H'\Omega - \Omega\, H'_{\rm eff}\big)P \tag{19c}$$

The Bloch equation is generally a *multi-state equation* that contains the information of a *system* of Schrödinger equations (11), corresponding to a number of target states. The equation can conveniently be used as the starting point for generating various perturbative schemes [58, 47]. It leads directly to a generalized form of the Rayleigh-Schrödinger perturbation expansion, and it can be used to generate the *linked-diagram expansion* (LDE). In the iterative form

$$\big[\Omega_n, H_0\big]P = \big(H'\Omega_{n-1} - \Omega_{n-1}\, H'_{{\rm eff},n}\big)P \tag{19d}$$

the equation can also be used to generate non-perturbative or "*all-order*" schemes, such as the *coupled-cluster approach* (CCA). Here, Ω_n and $H'_{{\rm eff},n} = PH'\Omega_{n-1}P$ (with $\Omega_0 = 1$) are the n:th approximations of the wave operator and the effective interaction, respectively. The commutator form of the Bloch equation makes it possible to work with a non-degenerate or "extended" model space, which is of particular importance for quasi-degenerate problems, as mentioned above.

2.2. Time-dependent perturbation theory

In time-dependent perturbation theory we start from the time-dependent Schrödinger equation

$$\mathrm{i}\frac{\partial}{\partial t}\,\big|\chi(t)\big\rangle = H\,\big|\chi(t)\big\rangle \tag{20}$$

We are here interested in states that are *stationary*, which implies that the state vector has the form

$$\big|\chi(t)\big\rangle = \big|\Psi\big\rangle\,\mathrm{e}^{-\mathrm{i}Et} \tag{21}$$

where E is the energy of the system and $|\Psi\rangle$ is the time-independent state vector. The latter is then a solution of the time-independent Schrödinger equation (2)

$$H\,|\Psi\rangle = E|\Psi\rangle \tag{22}$$

In the *interaction picture* (IP) [31] with the partitioning (12) the wave function is related to that of the Schrödinger picture by

$$\big|\chi_{\rm I}(t)\big\rangle = \mathrm{e}^{\mathrm{i}H_0 t}\big|\chi(t)\big\rangle \tag{23}$$

and the time-dependent Schrödinger equation becomes

$$\mathrm{i}\frac{\partial}{\partial t}\,\big|\chi_{\rm I}(t)\big\rangle = H'_{\rm I}(t)\,\big|\chi_{\rm I}(t)\big\rangle \tag{24}$$

The *time-evolution operator*, defined by

$$\big|\chi_{\rm I}(t)\big\rangle = U_{\rm I}(t,t_0)\,\big|\chi_{\rm I}(t_0)\big\rangle \tag{25}$$

then satisfies the equation

$$\mathrm{i}\frac{\partial}{\partial t}\,U_{\rm I}(t,t_0) = H'_{\rm I}(t)\,U_{\rm I}(t,t_0) \tag{26}$$

with the solution [31, Eq. 6.23]

$$U_{\rm I}(t,t_0) = 1 + \sum_{n=1}^{\infty}\frac{(-\mathrm{i})^n}{n!}\int_{t_0}^{t}\mathrm{d}^4x_n\cdots\int_{t_0}^{t}\mathrm{d}^4x_1\;T_{\rm D}\big[\mathcal{H}'_{\rm I}(x_n)\mathcal{H}'_{\rm I}(x_{n-1})\cdots\mathcal{H}'_{\rm I}(x_1)\big] \tag{27}$$

Here, $x = (t, \boldsymbol{x})$, $T_{\rm D}$ is the Dyson time-ordering operator, and $\mathcal{H}'_{\rm I}(x)$ is the perturbation *density*, related to the perturbation (12) by

$$H'_{\rm I}(t) = \int {\rm d}^3\boldsymbol{x}\, \mathcal{H}'_{\rm I}(t, \boldsymbol{x}) \tag{28}$$

In applying this formalism to perturbation theory, an *adiabatic damping* is added [31]

$$H'_{\rm I}(t) \to H'_{\rm I\gamma} = H'_{\rm I}\, {\rm e}^{-\gamma|t|}\,; \qquad U_{\rm I}(t, t_0) \to U_{\rm I\gamma}(t, t_0) \tag{29}$$

where γ is a small, positive number. This implies that as $t \to \pm\infty$ the eigenfunctions of H tend to eigenfunctions of H_0.

In QED the perturbation density due to the interaction between the electrons and the photon field is given by [71]

$$\mathcal{H}'_{\rm I}(x) = -e\hat{\psi}^\dagger_{\rm I}(x)\alpha^\mu A_\mu(x)\hat{\psi}_{\rm I}(x) \tag{30}$$

where e is the absolute value of the electronic charge, $\hat{\psi}^\dagger_{\rm I}(x)$, $\hat{\psi}_{\rm I}(x)$ are the electron-field operators in the interaction picture, A_μ the photon-field operator and α^μ are related to the standard Dirac matrices by $\alpha^\mu = (1, \boldsymbol{\alpha})$.

3. Green's function approach

In this section we shall essentially reproduce the derivation of the BS equation by Gell-Mann and Low, starting from Green's functions. We consider a two-particle system for which the Green's function is defined by [31, pp 64 and 116]

$$G(x'_1, x'_2; x_{10}, x_{20}) = -\frac{\big\langle 0_{\rm H}\big|T_{\rm D}[\hat{\psi}_{\rm H}(x'_1)\hat{\psi}_{\rm H}(x'_2)\hat{\psi}^\dagger_{\rm H}(x_{20})\hat{\psi}^\dagger_{\rm H}(x_{10})]\big|0_{\rm H}\big\rangle}{\langle 0_{\rm H}|0_{\rm H}\rangle} \tag{31}$$

Here, $|0_{\rm H}\rangle$ represents the vacuum state and $\hat{\psi}^\dagger_{\rm H}(x)$, $\hat{\psi}_{\rm H}(x)$ the electron-field operators, all in the *Heisenberg representation*. The latter are related to those in the interaction picture by

$$\hat{\psi}_{\rm H}(t, \boldsymbol{x}) = U(0, t)\, \hat{\psi}_{\rm I}(t, \boldsymbol{x})\, U(t, 0) \tag{32}$$

where U is the evolution operator (27). Transforming the Green's function to the interaction picture then yields [31, Eq. 8.9], [2, Eq. 16], [64, Eq. 259]

$$G(x'_1, x'_2; x_{10}, x_{20}) = -\frac{\big\langle 0_{\rm I}\big|T_{\rm D}[\hat{\psi}_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x'_2)U_{\rm I}(\infty, -\infty)\hat{\psi}^\dagger_{\rm I}(x_{20})\hat{\psi}^\dagger_{\rm I}(x_{10})]\big|0_{\rm I}\big\rangle}{\langle 0_{\rm I}|U_{\rm I}(\infty, -\infty)|0_{\rm I}\rangle} \tag{33}$$

Obviously, only fully contracted terms contribute to the vacuum expectation value. By applying *Wick's theorem* [31, p. 83] [47, Sect. 11.5], this can be represented in terms of *Feynman diagrams*. The denominator has the effect of eliminating the singularities of the numerator, in the Feynman picture represented by unlinked or disconnected diagrams, leading to [31, Eq. 9.5]

$$G(x'_1, x'_2; x_{10}, x_{20}) = -\big\langle 0_{\rm I}\big|T_{\rm D}[\hat{\psi}_{\rm I}(x'_1)\hat{\psi}_{\rm I}(x'_2)U_{\rm I}(\infty, -\infty)\hat{\psi}^\dagger_{\rm I}(x_{20})\hat{\psi}^\dagger_{\rm I}(x_{10})\big|0_{\rm I}\big\rangle_{\rm conn} \tag{34}$$

In contrast to the evolution operator (25), the Green's function is relativistically *covariant* in the sense that the integrations are performed over all space and time and the electron-field operators can represent particle (positive-energy) as well as hole (negative-energy) states. This also implies that, in the energy representation (fourier transform), the energy is conserved at all diagram vertices.

The Green's function can be expressed

$$G(x'_1, x'_2; x_{10}, x_{20}) = G_0(x'_1, x'_2; x_{10}, x_{20}) + \iiiint {\rm d}^4x_1\, {\rm d}^4x_2\, {\rm d}^4x_3\, {\rm d}^4\, x_4\; G_0(x'_1, x'_2; x_1, x_2)\, \mathcal{K}(x_1, x_2; x_3, x_4)\, G_0(x_3, x_4; x_{10}, x_{20}) \tag{35}$$

where $\mathcal{K}$ represents the interaction kernel of all connected diagrams and G_0 is the zeroth-order Green's function

$$\begin{aligned} G_0(x_1', x_2'; x_{10}, x_{20}) &= -\big\langle 0_{\rm I}\big|T_{\rm D}[\hat\psi_{\rm I}(x_1')\hat\psi_{\rm I}(x_2')\hat\psi_{\rm I}^\dagger(x_{20})\hat\psi_{\rm I}^\dagger(x_{10})]\big|0_{\rm I}\big\rangle \\ &= S_{\rm F}(x_1', x_{10})S_{\rm F}(x_2', x_{20}) \end{aligned} \tag{36}$$

with $S_{\rm F}$ being the Feynman *electron propagator* or zeroth-order single-electron Green's function, defined by

$$\mathrm{i}S_{\rm F}(x', x_0) = \big\langle 0_{\rm I}\big|T_{\rm D}[\hat\psi_{\rm I}(x')\hat\psi_{\rm I}^\dagger(x_0)]\big|0_{\rm I}\big\rangle \tag{37}$$

assuming the vacuum state be normalized. This is illustrated in Fig. 2. In operator form the Green's function can be expressed

$$G = G_0 + G_0\mathcal{K}G_0 \tag{38}$$

In some cases the kernel of the Green's function can be separated into two kernels

$$\mathcal{K} = \mathcal{K}_2 G_0 \mathcal{K}_1 \tag{39}$$

with no photon-field contractions between them. The kernel is then said to be *separable*. If a kernel cannot be separated further in this way, it is said to be *non-separable* [2]. The complete kernel can then be expressed

$$\mathcal{K} = \kappa + \kappa G_0 \kappa + \kappa G_0 \kappa G_0 \kappa + \cdots \tag{40}$$

where κ represents all *non-separable* kernels. This leads to the *Dyson equation* for the Green's function

$$G = G_0 + G_0 \kappa G \tag{41}$$

illustrated in Fig. 3.

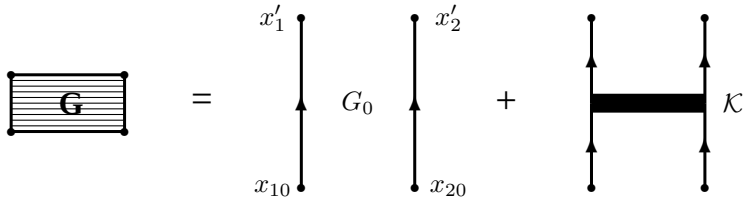


Fig. 2. Graphical representation of the two-particle Green's function (38). $\mathcal{K}$ represents *all* interactions between the electrons.

Bethe and Salpeter as well as Gell-Mann and Low argue that a related equation can be set up for the two-electron bound-state wave function. In that case the first (inhomogeneous) term on the rhs does not contribute, since that is in their formulation composed of *free-electron* propagators, and the bound-state wave function does not have any such components. This leads to the *homogeneous* equation

$$\Psi(x_1', x_2') = \iiiint \mathrm{d}^4x_1\,\mathrm{d}^4x_2\,\mathrm{d}^4x_3\,\mathrm{d}^4x_4\; G_0(x_1', x_2'; x_1, x_2)\,\kappa(x_1, x_2; x_3, x_4)\,\Psi(x_3, x_4) \tag{42}$$

or in short-hand notations

$$\Psi = G_0\,\kappa\,\Psi \tag{43}$$

[2] What we here refer to as "separable" and "non-separable" are often referred to as "reducible" and "irreducible". Since the latter terms have recently been used also with a different interpretation, we avoid them here.

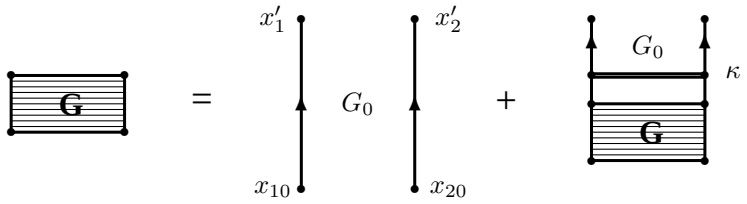


Fig. 3. Graphical representation of the Dyson equation (41) for the two-particle Green's function. κ represents the *non-separable* interactions between the electons.

This is the original form of the Bethe-Salpeter equation [1, Eq. 11a], [2, Eq. 37]. It should be noted that this wave function contains *individual times for the two particles*. This reflects one of the problems referred to in the Introduction. The relative time between the particles does not correspond to any physical quantity and leads to spurious solutions. There are several ways of eliminating the extra time dependence in a covariant way. Sucher [38], following Salpeter [18], integrates the fourier transform over the relative energy, which leads to a Schrödinger-like form with a single time/energy dependence of the type (8) given above. This reduction can be done without loosing any physical content of the original equation [15, 16, 32, 17]. In the following sections we shall derive an equivalent equation in a different way.

Our notations here differ from those used by Bethe-Salpeter and Gell-Mann–Low. The Green's function (31) is in their works denoted by $K(12,34)$ and referred to as the "*amplitude function for the propagation of the particles*" by Bethe-Salpeter [1] and as the "*two-body kernel*" by Gell-Mann–Low [2, Eq. 11]. Our "non-separable kernel" κ is by BS denoted by $\bar{G}$ and referred to as "*irreducible graphs*" and by GML denoted by G and referred to as the "*interaction function*".

4. Covariant evolution operator approach

4.1. Definitions

In the following sections we shall derive the Bethe-Salpeter equation, starting from the covariant form of the evolution operator [64]. This will demonstrate the relation between the BS equation and standard many-body perturbation theory (MBPT) in a clear way. In the present section we shall first review the basics of the evolution-operator method and in the next section use that method for deriving the BS equation. This will directly lead to the Schrödinger-like form (8).

According to the Gell-Mann–Low theorem [2, 31, p. 61] the time-independent state vector (21) can in the case of a single target state be expressed in intermediate normalization (IN) (14) as

$$|\mathbf{\Psi}\rangle = |\chi(0)\rangle = \lim_{\gamma\to 0} \frac{U_\gamma(0,-\infty)\big|\Psi_0\big\rangle}{\langle\Psi_0|U_\gamma(0,-\infty)|\Psi_0\rangle} \tag{44}$$

where U_γ is the evolution operator (29) and $|\Psi_0\rangle$ is the time-independent zeroth-order state (15). (From now on we work in the interaction picture and leave out the subscript "I".) $|\mathbf{\Psi}\rangle$ is an eigenvector of the Hamiltonian $H_0 + H'$

$$(H_0 + H')\,|\mathbf{\Psi}\rangle = E\,|\mathbf{\Psi}\rangle \tag{45}$$

where H' is in our case the electron-field interaction density (30), integrated over the space. Since this perturbation represents an *uncontracted* photon, the state vector $|\mathbf{\Psi}\rangle$ will generally lie in an *extended Fock space*, where the number of photons is not conserved.

The GML formula can be generalized to a general multi-dimensional model space [64, Eq. 110]

$$|\mathbf{\Psi^\alpha}\rangle = \lim_{\gamma\to 0} \frac{N^\alpha U_\gamma(0,-\infty)|\Phi^\alpha\rangle}{\langle\Phi^\alpha|U_\gamma(0,-\infty)|\Phi^\alpha\rangle}\,; \qquad (\alpha = 1,2,\cdots d) \tag{46}$$

where the vector $|\Phi^\alpha\rangle$ is defined

$$|\Phi^\alpha\rangle = \lim_{\gamma\to 0}\lim_{t\to-\infty} |\chi^\alpha(t)\rangle \tag{47}$$

This state is generally distinct from the zeroth-order state (15) in intermediate normalization. Since the state (47) generally does not satisfy IN, a normalization constant N^α is inserted.

$$U_{\rm Noncov}(t',t_0) = 1 +$$

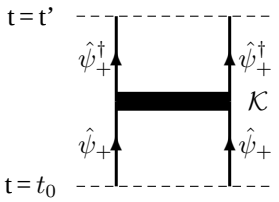
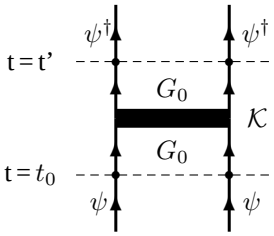


Fig. 4. Graphical representation of the non-covariant evolution operator (48). The time evolution occurs only in the positive direction.

$$U_{\rm Cov}(t',t_0) = 1 +$$



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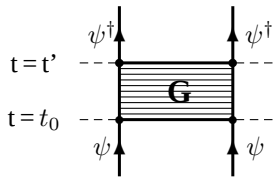

Fig. 5. Graphical representation of the covariant evolution (49) (left). Here, time evolution can occur in the positive as well as the negative direction. The right part of the figure depicts the relation to the two-time Green's function (50).

For a two-electron system the *non-covariant* evolution operator (25) can in analogy with the Green's function (38) be expressed

$$U_{\rm Noncov}(t',t_0) = 1 + \hat\psi_+^\dagger(x_1')\hat\psi_+^\dagger(x_2')\,\mathcal{K}\,\hat\psi_+(x_{20})\hat\psi_+(x_{10}) \tag{48}$$

where again $\mathcal{K}$ represents the kernel of all fully contracted (separable and non-separable) interactions and $\hat\psi_+^\dagger$, $\hat\psi_+$ the positive-energy part of the electron-field operators. This is illustrated in Fig. 4. In contrast to the Green's function above, the evolution operator (27) has a single initial time $t = t_0$ and a single final time $t = t'$. The time integration is performed from $t = t_0$ to $t = t'$ — only in the positive direction — which implies that the operator is *not relativistically covariant*.

A fully covariant form of the evolution operator that is applicable to relativistic problems can be obtained by inserting electron propagators in the non-covariant expression, as indicated in Fig. 5 (left), corresponding to the expression [66, 64, Sect. 5]

$$U_{\rm Cov}(t',t_0) = 1 + \iiiint {\rm d}^3\boldsymbol{x}_1'\,{\rm d}^3\boldsymbol{x}_2'\,{\rm d}^3\boldsymbol{x}_{10}\,{\rm d}^3\boldsymbol{x}_{20}\;\hat\psi^\dagger(x_1')\hat\psi^\dagger(x_2')\,G_0\mathcal{K}G_0\,\hat\psi(x_{20})\hat\psi(x_{10}) \tag{49}$$

leaving out the integrations over the coordinates of $\mathcal{K}$ (see Eq. 35). It then follows from relation (38) that the covariant evolution operator is related to the *two-time* Green's function (where all initial and

all final times are equal) by

$$U_{\rm Cov}(t',t_0) = \iiiint {\rm d}^3\boldsymbol{x}'_1\,{\rm d}^3\boldsymbol{x}'_2\,{\rm d}^3\boldsymbol{x}_{10}\,{\rm d}^3\boldsymbol{x}_{20}\;\hat\psi^\dagger(x'_1)\hat\psi^\dagger(x'_2)\,G(x'_1,x'_2;x_{10},x_{20})\,\hat\psi(x_{20})\hat\psi(x_{10}) \tag{50}$$

as illustrated in Fig. 5 (right).

From the relations [64, Eq. 193 (note misprints)]

$$\begin{aligned}\int {\rm d}^3\boldsymbol{x}_0\,{\rm i}S_{\rm F}(x,x_0)\,\hat\psi(x_0) &= \Theta(t-t_0)\,\hat\psi_+(x) - \Theta(t_0-t)\,\hat\psi_-(x)\\ \int {\rm d}^3\boldsymbol{x}\,\hat\psi^\dagger(x)\,{\rm i}S_{\rm F}(x,x_0) &= \Theta(t-t_0)\,\hat\psi^\dagger_+(x_0) - \Theta(t_0-t)\,\hat\psi^\dagger_-(x_0)\end{aligned} \tag{51}$$

it follows directly that the form (49) is equivalent to the non-covariant form (48), when only particle states are involved. That the former in addition is relativistically covariant follows from the fact that *the electron-field operators can represent particle as well as hole states and the internal time integrations are performed over all times*— in the positive as well as the negative direction. From now on we shall work only with the covariant form of the evolution operator and leave out the subscript "$_{\rm Cov}$".

In using the evolution operator in perturbation theory, we assume that we operate to the far right on positive-energy states in the model space. Then, as shown in Appendix B, we can eliminate the rightmost zeroth-order Green's function and set the initial time to $t_0 = -\infty$. We shall also assume that the limit of the adiabatic damping $\gamma \to 0$ is taken.

The covariant evolution operator is closely related to the Green's function—the main difference being that the Green's function is a *function*, while the evolution operator is an *operator*. The poles of the Green's function (in the energy representation) correspond to the energies of the system, while the procedure gives no direct information about the wave function. The covariant evolution operator, on the other hand, contains information about the energy as well as the wave function.

4.2. Model-space contributions

Even after eliminating unlinked or disconnected contributions in Eq. (34), the evolution operator may contain (quasi)singularities, namely when the intermediate state of a separable kernel lies in the model space and is degenerate or nearly degenerate (quasi-degenerate) with the initial state. As mentioned, a kernel is said to be *separable*, if it can be separated into two kernels with no photon contractions between them. Singularities appear only for separable interactions. In the covariant-evolution-operator approach these singularities are eliminated by introducing a *reduced evolution operator* $\widetilde{U}(t,-\infty)$ [66, 64, Eq. 116], defined by

$$U(t,-\infty)P = P + \widetilde{U}(t,-\infty)P\cdot PU(0,-\infty)P \tag{52}$$

Here, the last term is a product of two operators that evolve *independently* from initial states in the model space ($t=-\infty$), which is indicated by the "dot". Note also that the last factor has the final time $t=0$ and hence is time independent. This situation should be distinguished from the case where two operators are "coupled" and operate "in succession"

$$U(t,t_0) = U(t,t")\,U(t",t_0) \tag{53}$$

This distinction will be important for the following treatment.

Normally, we shall assume that the initial time in the evolution operator is $t_0=-\infty$, and in cases where there is no risk for ambiguity we shall leave that out from the operator, so that

$$U(t) = U(t,-\infty)$$

The definition (52) will then be written

$$\boxed{U(t)P = P + \widetilde{U}(t)P \cdot PU(0)P} \tag{54}$$

We also introduce the notation $U'(t) = U(t) - 1$, which yields in place of the definition (54)

$$\widetilde{U}(t)P = U'(t)P - \widetilde{U}(t)P \cdot PU'(0)P \tag{55}$$

Here, the last term is the *counterterm*

$$\boxed{C(t) = -\widetilde{U}(t)P \cdot PU'(0)P} \tag{56}$$

which removes the (quasi)singularities. This can also be expressed

$$C(t) = -\widetilde{U}(t)P \cdot P\widetilde{U}(0)P - \widetilde{U}(t)P \cdot P\widetilde{U}(0)P \cdot P\widetilde{U}(0)P - \cdots \tag{57}$$

After removing a singularity, there is normally a non-vanishing remainder (M), referred to as the *model-space contribution* (MSC), defined by

$$\boxed{M(t) = \widetilde{U}(t)P - \bar{U}(t)P} \tag{58}$$

and further discussed in the Appendices. The new operator $\bar{U}$ (*"U-bar"*) is defined as the evolution operator with *all model-space states removed*. (The MSC is analogous to the *reference-state contribution*, appearing in the S-matrix formalism, where the effect normally appears only when the intermediate states is equal to the reference or initial state. In our formalism with an extended model space the effect can appear also for other model-space states, and we prefer the more general term.) It should be noted that the counterterms also remove quasi-singularities, due to quasi-degenerate states that are included in the model space. This can be of vital importance for the convergence of the procedure.

As discussed in Appendix C, the model-space contributions are of *two kinds*. The first kind appears for all interactions, even if they are time or energy independent, while the second kind appears only for time- or energy-dependent interactions. The first kind appears also in standard time-independent perturbation theory and corresponds to so-called *folded diagrams* of MBPT [47, 64, Fig. 5].

4.3. The wave operator and effective interaction

As mentioned previously, the evolution operator (27) with the perturbation density (30) can contain uncontracted photon operators, which implies that it operates in a general *Fock space*, where the number of virtual photons is not conserved. We then separate the covariant evolution operator (49) into

$$U(t) = PU(t) + \boldsymbol{Q}U(t) \tag{59}$$

where $\boldsymbol{Q} = 1 - P$ is operating in the general Fock space, while P is the projection operator for the model space, confined to the restricted Hilbert space with no uncontracted photon. This leads with the definition (54) of the reduced evolution operator for $t = 0$ to the *factorization theorem* [64, Eq. 121]

$$\boxed{U(0)P = \left[1 + \boldsymbol{Q}\widetilde{U}(0)\right]P \cdot PU(0)P} \tag{60}$$

where the first factor on rhs is regular. Inserted in the GML formula (46), this yields

$$|\boldsymbol{\Psi}^{\boldsymbol{\alpha}}\rangle = \left[1 + \boldsymbol{Q}\widetilde{U}(0)\right]|\Psi_0^\alpha\rangle \tag{61}$$

where Ψ_0^α is the zeroth-order wave function (ZOWF) (15) in intermediate normalization

$$|\Psi_0^\alpha\rangle = P|\boldsymbol{\Psi}^{\boldsymbol{\alpha}}\rangle = \frac{N^\alpha PU(0)|\Phi^\alpha\rangle}{\langle\Phi^\alpha|U(0)|\Phi^\alpha\rangle} \tag{62}$$

The square bracket above is the *wave operator*

$$\begin{aligned} \boldsymbol{\Omega} &= 1 + \boldsymbol{Q}\widetilde{U}(0) \\ |\boldsymbol{\Psi}^{\boldsymbol{\alpha}}\rangle &= \boldsymbol{\Omega}\,|\Psi_0^\alpha\rangle \end{aligned} \tag{63}$$

The result here is a direct consequence of the generalized Gell-Mann–Low theorem and the definition of the reduced evolution operator.

As mentioned, with the perturbation (30) the wave function $\boldsymbol{\Psi}^\alpha$ lies generally in a Fock space where the number of (virtual) photons is not conserved. But we are interested here in the case where all photon operators are fully contracted, and for that purpose we project the equation on the restricted Hilbert space without uncontracted photon operators

$$\mathcal{P}|\boldsymbol{\Psi}\rangle = \mathcal{P}\big[1 + Q\widetilde{U}(0)\big]|\Psi_0^\alpha\rangle \tag{64}$$

or

$$|\Psi^\alpha\rangle = \big[1 + Q\widetilde{U}(0)\big]|\Psi_0^\alpha\rangle \tag{65}$$

where $|\Psi^\alpha\rangle = \mathcal{P}|\boldsymbol{\Psi}^{\boldsymbol{\alpha}}\rangle$ is the projected wave function on the restricted Hilbert space and $Q = \mathcal{P}\boldsymbol{Q}$ is the conventional projection operator for the complementary space (outside the model space). The wave operator in this space is

$$\boxed{\Omega = \mathcal{P}\boldsymbol{\Omega} = 1 + Q\widetilde{U}(0)} \tag{66}$$

In IN (14) the wave operators satisfy in both spaces the relation (16)

$$P\boldsymbol{\Omega}P = P\Omega P = P. \tag{67}$$

The *effective interaction* (19b) is in this formalism given by [64, Eq. 130]

$$\boxed{H'_{\rm eff} = P\Big[\mathrm{i}\frac{\partial}{\partial t}\widetilde{U}(t)\Big]_{t=0}P} \tag{68}$$

5. Connection to the Bethe-Salpeter equation

5.1. Expansion of the wave operator

We know from the generalized Gell-Mann–Low relation (46) that the state vector $|\boldsymbol{\Psi}^\alpha\rangle$ in the extended Fock space satisfies a Schrödinger-like equation (45) with the Hamiltonian $H = H_0 + H'$, where H' is the perturbation (30). We now want to find the corresponding equation for the projected state $|\Psi^\alpha\rangle = \mathcal{P}|\boldsymbol{\Psi}^\alpha\rangle$ in the restricted space with no uncontracted photons, and we shall see in this section that this leads to the *Bethe-Salpeter equation*.

We shall start with the exchange of a sequence of separable covariant single photons between the electrons, which can then be generalized to other interactions, leading to the full equation. This will first be done for a degenerate model space and then extended to the general case.

As shown in Appendix B (Eq. 162), the contribution to the wave operator due the exchange of a single photon, operating to the right on a state of the energy $\mathcal{E}$, is

$$\Omega^{(1)}P = Q\widetilde{U}^{(1)}(0,\mathcal{E})P = \Gamma_Q(\mathcal{E})V(\mathcal{E})P \tag{69}$$

and the corresponding contribution to the effective Hamiltonian $H^{(1)}_{\rm eff}(\mathcal{E}) = PV(\mathcal{E})P$. Here, $\Gamma_Q(\mathcal{E})$ is the "reduced" resolvent (163) and $V(\mathcal{E})$ is the effective single-photon potential (165),

Similarly, it is demonstrated in Appendix C (Eq. 182) that the contribution to the evolution operator from *two* separable single-photon interactions is

$$\Omega^{(2)}P = Q\widetilde{U}^{(2)}(0)P = \Gamma_Q V\Omega^{(1)}P + \frac{\delta\Omega^{(1)}}{\delta\mathcal{E}} * H^{(1)}_{\rm eff} \tag{70}$$

where the last term represents the *model-space contribution* (MSC) (58). The asterisk is introduced here only to indicate that there is a cancelled singularity at that position, which is of importance for the further treatment, as discussed in the Appendices.) The contribution to the effective Hamiltonian (184) due to two-photon exchange is

$$H^{(2)}_{\rm eff} = PV\Omega^{(1)}P + \frac{\delta H^{(1)}_{\rm eff}}{\delta\mathcal{E}} * H^{(1)}_{\rm eff} \tag{71}$$

The last term is the MSC to the effective interaction, and if the model space is degenerate with the energy E_0 that term becomes

$$\frac{\partial H^{(1)}_{\rm eff}}{\partial\mathcal{E}} * H^{(1)}_{\rm eff} = P\frac{\partial V(\mathcal{E})}{\partial\mathcal{E}}\Big|_{E_0} PV(E_0)P \tag{72}$$

This corresponds to the "reference-state contribution", discussed in connection with the S-matrix treatment of two-photon exchange [72, 73].

The treatment above will now be generalized to all orders as a first step towards deriving the full BS equation. We start with the covariant evolution operator (49) $U(t) = U(t,-\infty)$ and the reduced evolution operator (55)

$$\widetilde{U}(t)P = U'(t)P - \widetilde{U}(t)P \cdot PU'(0)P \tag{73}$$

where $U' = U - 1$. Note that only the first factor in the product is time dependent (see. Eq. 172). Note also the appearance of the "dots" in this expression. The significance of the dot is discussed in relation to the definition (52).

In the following we shall leave out the prime on U' and normally also the time arguments. The reduced evolution operator (73) then becomes

$$\widetilde{U}P = UP - \widetilde{U}P \cdot PUP$$

where

$$\boxed{C = -\widetilde{U}P \cdot PUP} \tag{74}$$

is the *counterterm* (56). For $t = 0$ the evolution operator is with these notations given by

$$U = \Gamma V + \Gamma V\Gamma V + \Gamma V\Gamma V\Gamma V + \cdots \tag{75}$$

where $\Gamma = \Gamma(\mathcal{E})$ is the resolvent (146), and the "*U-bar*" operator (58), with all intermediate model-space states removed, by

$$\bar{U} = \Gamma V + \Gamma V\Gamma_Q V + \Gamma V\Gamma_Q V\Gamma_Q V + \cdots \tag{76}$$

We introduce a special symbol for the time derivative at time $t = 0$

$$\boxed{\dot{A} = \mathrm{i}\frac{\partial A}{\partial t}\Big|_{t=0}} \tag{77}$$

Since the evolution operator (161, 172) has the time dependence

$$U(t,\mathcal{E}) = \mathrm{e}^{-\mathrm{i}t(\mathcal{E}-H_0)}\, U(0,\mathcal{E})$$

it follows that the time derivation eliminates the denominator of the first (leftmost) resolvent, so that

$$\begin{aligned} \dot{U} &= V + V\Gamma V + V\Gamma V\Gamma V + \cdots \\ \dot{\tilde{U}} &= V + V\Gamma_Q V + V\Gamma_Q V\Gamma_Q V + \cdots \end{aligned} \tag{78}$$

The *effective interaction* $H'_{\rm eff}$ (68) is with this notation given by

$$\boxed{H'_{\rm eff} = P\dot{\tilde{U}}P} \tag{79}$$

We also introduce the corresponding *"H-bar"* operator with no intermediate model-space states

$$\bar{H}'_{\rm eff} = P\dot{\bar{U}}P \tag{80}$$

We recall the definition (58) of the model-space contribution (MSC)

$$\tilde{U}P = \bar{U}P + M \tag{81}$$

and can easily derive the identities (valid for arbitrary times)

$$UP = \bar{U}P + \bar{U}\,PUP = \bar{U}P + \tilde{U}\,PUP - M\,PUP \tag{82}$$

$$\bar{U}P = UP - U\,PUP + U\,PUP\,PUP - \cdots \tag{83}$$

Then the reduced evolution operator (73) becomes

$$\tilde{U}P = UP + C = \bar{U}P + \tilde{U}\,PUP - \tilde{U}P\cdot PUP - M\,PUP \tag{84}$$

Here, the last three terms represent the MSC

$$M = \tilde{U}P - \bar{U}P = \tilde{U}\,PUP - \tilde{U}P\cdot PUP - M\,PUP \tag{85}$$

which leads to the series expansion

$$\tilde{U}P = \bar{U}P + \big(\tilde{U}\,PUP - \tilde{U}P\cdot PUP\big)\big(1 - PUP + PUP\,PUP + \cdots\big) \tag{86}$$

With the identity (83) this becomes

$$\boxed{\tilde{U}P = \bar{U}P + \big(\tilde{U}\,P\bar{U}P - \tilde{U}P\cdot P\bar{U}P\big)} \tag{87}$$

which is an exact expression also for a quasi-degenerate model space. It can be expanded as

$$\tilde{U}P = \bar{U}P + \big(\bar{U}\,P\bar{U}P - \bar{U}P\cdot P\bar{U}P\big) + \big(\bar{U}\,P\bar{U}P - \bar{U}P\cdot P\bar{U}P\big)\big(P\bar{U}P - \cdot P\bar{U}P\big) + \cdots \tag{88}$$

As discussed in Appendix C, the result (87) can be expressed

$$\tilde{U}P = \bar{U}P + \frac{\delta\tilde{U}}{\delta\mathcal{E}} * P\dot{\bar{U}}P = \bar{U}P + \frac{\delta\tilde{U}}{\delta\mathcal{E}} * \bar{H}'_{\rm eff} \tag{89}$$

where $\delta\mathcal{E}$ is the change in the model-space energy, represented by the "dot", $\delta\tilde{U}$ is the corresponding change in $\tilde{U}$, and $\bar{H}'_{\rm eff}$ is the "H-bar" operator (80). In the case of complete degeneracy this becomes

$$\tilde{U}P = \bar{U}P + \frac{\partial\tilde{U}}{\partial\mathcal{E}}\Big|_{\mathcal{E}=E_0} * \bar{H}'_{\rm eff} \tag{90}$$

Introducing the*"Omega-bar"* operator $\bar{\Omega}$ (with no intermediate model-space states) in analogy with the wave operator (66)

$$\bar{\Omega}P = P + Q\bar{U}P = P + \Gamma_Q V P + \Gamma_Q V \Gamma_Q V P + \cdots \tag{91}$$

we can express the relations above as

$$\boxed{\Omega P = \bar{\Omega}P + \frac{\delta\Omega}{\delta\mathcal{E}} * \bar{H}'_{\rm eff} \Rightarrow \bar{\Omega}P + \frac{\partial\Omega}{\partial\mathcal{E}}\Big|_{\mathcal{E}=E_0} * \bar{H}'_{\rm eff}} \tag{92}$$

The second term is here consequently an exact expression for the entire model-space contribution to the wave operator. This is in agreement with the three-photon result (193).

By taking the time derivative of the relation (87), using the relations above, we obtain similarly

$$\boxed{H'_{\rm eff} = \bar{H}'_{\rm eff} + \frac{\delta H'_{\rm eff}}{\delta\mathcal{E}} * \bar{H}'_{\rm eff} \Rightarrow \bar{H}'_{\rm eff} + \frac{\partial H'_{\rm eff}}{\partial\mathcal{E}}\Big|_{\mathcal{E}=E_0} * \bar{H}'_{\rm eff}} \tag{93}$$

The second term represents here the model-space contribution to the effective interaction. This result agrees also with the third-order result (195).

From the results above we conjecture that the wave operator can at complete degeneracy alternatively be expressed

$$\Omega P = \bar{\Omega}P + \frac{\partial\bar{\Omega}}{\partial\mathcal{E}} * H'_{\rm eff} + \frac{1}{2}\frac{\partial^2\bar{\Omega}}{\partial\mathcal{E}^2} * \big(H'_{\rm eff}\big)^2 + \frac{1}{3!}\frac{\partial^3\bar{\Omega}}{\partial\mathcal{E}^3} * \big(H'_{\rm eff}\big)^3 + \cdots = \bar{\Omega}P + \sum_{n=1}^{\infty}\frac{1}{n!}\frac{\partial^n\bar{\Omega}}{\partial\mathcal{E}^n} * \big(H'_{\rm eff}\big)^n \tag{94}$$

with all derivatives taken at $\mathcal{E} = E_0$, and we shall now prove this relation by showing that it is compatible with the results (92) and (93), which we have rigorously derived. This equation contains eliminated singularities, indicated by the asterisks. These expressions are obtained by considering a quasi-degenerate case, letting the energy separation tend to zero. In order to form a new derivative, it is—as discussed in the Appendices, particularly Appendix E—necessary first to lift the degeneracy and then let the separation tend to zero in a *single* step. Using the rules developed we find for instance

$$\frac{\partial}{\partial\mathcal{E}}\Big(\frac{\partial\bar{\Omega}}{\partial\mathcal{E}} * H'_{\rm eff}\Big) \;\Rightarrow\; \frac{\delta}{\delta\mathcal{E}}\Big(\frac{\delta\bar{\Omega}}{\delta\mathcal{E}} * H'_{\rm eff}\Big) \Rightarrow \frac{1}{2}\frac{\partial^2\bar{\Omega}}{\partial\mathcal{E}^2} * H'_{\rm eff} + \frac{\partial\bar{\Omega}}{\partial\mathcal{E}} * \frac{\partial H'_{\rm eff}}{\partial\mathcal{E}} \tag{95}$$

$$\frac{\partial}{\partial\mathcal{E}}\Big(\frac{1}{2}\frac{\partial^2\bar{\Omega}}{\partial\mathcal{E}^2} * \big(H'_{\rm eff}\big)^2\Big) \;\Rightarrow\; \frac{\delta}{\delta\mathcal{E}}\Big(\frac{\delta^2\bar{\Omega}}{\delta\mathcal{E}^2} * \big(H'_{\rm eff}\big)^2\Big)$$
$$\Rightarrow\; \frac{1}{3!}\frac{\partial^3\bar{\Omega}}{\partial\mathcal{E}^3} * \big(H'_{\rm eff}\big)^2 + \frac{1}{2}\frac{\partial^2\bar{\Omega}}{\partial\mathcal{E}^2} * \frac{\partial H'_{\rm eff}}{\partial\mathcal{E}} * H'_{\rm eff} \tag{96}$$

Note that in the second example the two $H'_{\rm eff}$ operators have in the quasi-degenerate case different energy parameters, and therefore only one of them is affected by the derivation.

Generalizing these rules, we can evaluate the derivative of the wave operator (94)

$$\begin{aligned}\frac{\partial\Omega}{\partial\mathcal{E}} &= \frac{\partial\bar{\Omega}}{\partial\mathcal{E}} + \frac{1}{2}\frac{\partial^2\bar{\Omega}}{\partial\mathcal{E}^2} * H'_{\rm eff} + \frac{1}{3!}\frac{\partial^3\bar{\Omega}}{\partial\mathcal{E}^3} * \big(H'_{\rm eff}\big)^2 + \cdots \\ &+ \frac{\partial\bar{\Omega}}{\partial\mathcal{E}} * \frac{\partial H'_{\rm eff}}{\partial\mathcal{E}} + \frac{1}{2}\frac{\partial^2\bar{\Omega}}{\partial\mathcal{E}^2} * \frac{\partial H'_{\rm eff}}{\partial\mathcal{E}} * H'_{\rm eff} + \frac{1}{3!}\frac{\partial^3\bar{\Omega}}{\partial\mathcal{E}^3} * \frac{\partial H'_{\rm eff}}{\partial\mathcal{E}} * (H'_{\rm eff})^2 + \cdots\end{aligned} \tag{97}$$

or

$$\frac{\partial\Omega}{\partial\mathcal{E}} = \sum_{n=1}^{\infty}\frac{1}{n!}\frac{\partial^n\bar{\Omega}}{\partial\mathcal{E}^n} * \Big[\big(H'_{\rm eff}\big)^{n-1} + \frac{\partial H'_{\rm eff}}{\partial\mathcal{E}} * (H'_{\rm eff})^{n-1}\Big] \tag{98}$$

We now insert this expression into the equation (92), which yields

$$\frac{\partial\Omega}{\partial\mathcal{E}} * \bar{H}'_{\rm eff} = \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n \bar{\Omega}}{\partial \mathcal{E}^n} * \left[\left(H'_{\rm eff}\right)^{n-1} * \bar{H}'_{\rm eff} + \frac{\partial H'_{\rm eff}}{\partial \mathcal{E}} * (H'_{\rm eff})^{n-1} * \bar{H}'_{\rm eff} \right] \tag{99}$$

or, using the relation (93),

$$\boxed{\Omega P = \bar{\Omega} P + \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n \bar{\Omega}}{\partial \mathcal{E}^n} * \left(H'_{\rm eff}\right)^n} \tag{100}$$

This is identical to the conjectured relation (94) and therefore completes the proof. The sum represents by definition the model-space contribution (MSC).

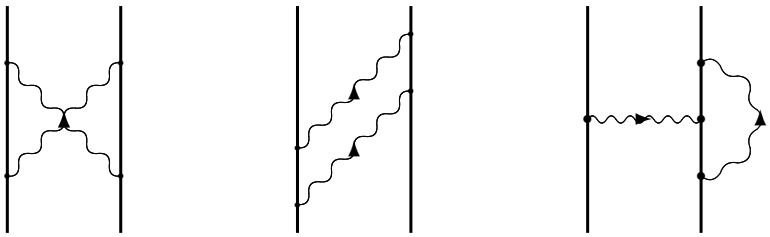

Fig. 6. Examples of non-separable two-photon interactions.

5.2. Derivation of the Bethe-Salpeter equation. Degenerate model space.

The previous treatment has been based upon the Hamiltonian $H = H_0 + V(E)$, where $V(E)$ is the potential due to the exchange of a single covariant photon. But the process can be repeated in exactly the same way, if we include *all non-separable multi-photon interactions*. A non-separable interaction is defined as an interaction that cannot be represented by two or more simpler interactions in the way treated here. Two photons—crossing or noncrossing— that overlap in time represent non-separable two-photon interactions (see Fig. 6, c.f. also Ref. [1, Fig. 1]). These can also include the radiative self-energy and vertex corrections. In a similar way non-separable three-, four-,... photon interactions can be defined. Therefore, in the following we replace the single-photon potential V by the general potential due to all non-separable interactions

$$\mathcal{V}(E) = V(E) + V_2(E) + V_3(E) + \cdots \tag{101}$$

As discussed in the Appendices, when operating on a state of energy $\mathcal{E}$, the energy parameter of $\bar{\Omega}P$ is equal to that energy, i.e.,

$$\bar{\Omega} F(\mathcal{E}) = \bar{\Omega}(\mathcal{E}) F(\mathcal{E}) \tag{102}$$

For a degenerate model space of energy E_0 this means that

$$\bar{\Omega} P = \bar{\Omega}(E_0) P = P + \Gamma_Q(E_0) \mathcal{V}(E_0) + \cdots \tag{103}$$

The model functions are eigenfunctions of the effective Hamiltonian (17), and for a degenerate model space (of energy E_0) they are eigenfunctions also of the effective interaction (19b),

$$H'_{\rm eff} |\Psi_0^\alpha\rangle = \Delta E^\alpha |\Psi_0^\alpha\rangle \tag{104}$$

where $\Delta E^\alpha = E^\alpha - E_0$. Operating with the operator equation (100) directly on the model state $|\Psi_0^\alpha\rangle$ then leads to the Taylor expansion

$$\Omega|\Psi_0^\alpha\rangle = \Big[\bar{\Omega}(E_0) + \frac{\partial\bar{\Omega}}{\partial\mathcal{E}}\Big|_{E_0}\Delta E^\alpha + \frac{1}{2}\frac{\partial^2\bar{\Omega}}{\partial\mathcal{E}^2}\Big|_{E_0}(\Delta E^\alpha)^2 + \frac{1}{3!}\cdots\Big]\big|\Psi_0^\alpha\big\rangle = \bar{\Omega}(E^\alpha)|\Psi_0^\alpha\rangle \tag{105}$$

This implies that *the MSC term shifts the energy parameter of the resolvent as well as that of the potential from the unperturbed energy E_0 to the exact energy E^α*. But $\bar{\Omega}(E^\alpha)\,\Psi_0^\alpha$ with the energy parameter equal to the full energy for the state Ψ^α is also identical to the *Brillouin-Wigner expansion* (9),

$$\bar{\Omega}(E^\alpha)|\Psi_0^\alpha\rangle = \Big[1 + \frac{Q}{E^\alpha - H_0}\,\mathcal{V}(E^\alpha) + \frac{Q}{E^\alpha - H_0}\,\mathcal{V}(E^\alpha)\frac{Q}{E^\alpha - H_0}\,\mathcal{V}(E^\alpha) + \cdots\Big]\big|\Psi_0^\alpha\big\rangle \tag{106}$$

which represents the full wave function, i.e.,

$$\boxed{\bar{\Omega}(E^\alpha)|\Psi_0^\alpha\rangle = \Omega|\Psi_0^\alpha\rangle} \tag{107}$$

This implies that the relation (100) essentially represents *the link between the Rayleigh-Schrödinger and the Brillouin-Wigner expansions for an energy-dependent interaction* and at the same time *the link between the MBPT approaches and the Bethe-Salpeter equation* (indicated by the arrows in the diagram of Fig. 1).

The BW expansion (106) can be expressed

$$\Omega|\Psi_0^\alpha\rangle = |\Psi_0^\alpha\rangle + \Gamma_Q(E^\alpha)\mathcal{V}(E^\alpha)\Omega|\Psi_0^\alpha\rangle \tag{108}$$

or

$$(E^\alpha - H_0)\,Q|\Psi^\alpha\rangle = Q\mathcal{V}(E^\alpha)|\Psi^\alpha\rangle \tag{109}$$

From the relation (93) it can be shown in analogy with the relation (100)

$$H'_{\rm eff} = \bar{H}'_{\rm eff} + \sum_{n=1}^{\infty}\frac{1}{n!}\,\frac{\partial^n\bar{H}'_{\rm eff}}{\partial\mathcal{E}^n} * \big(H'_{\rm eff}\big)^n \tag{110}$$

With the definitions (80) and (91) this leads to

$$\bar{H}'_{\rm eff} = P\mathcal{V}(E_0)\,\bar{\Omega}(E_0)P \tag{111}$$

and in analogy with the relation (105) to

$$H'_{\rm eff} = P\mathcal{V}(E^\alpha)\,\bar{\Omega}(E^\alpha)P = P\mathcal{V}(E^\alpha)\,\Omega P \tag{112}$$

This leads together with Eq. (109) to the final equation

$$\boxed{(E^\alpha - H_0)\,|\Psi^\alpha\rangle = \mathcal{V}(E^\alpha)\,|\Psi^\alpha\rangle} \tag{113}$$

This is the Bethe-Salpeter equation for energy-dependent interactions in the Schrödinger-like form (8). This can be solved iteratively as the standard Bloch equation (19d).

We have now confirmed that the Schrödinger equation (45)*, obtained directly from the generalized Gell-Mann–Low relation in the extended Fock space with the perturbation density* (30)*, corresponds in the projected Hilbert space with no uncontracted photons to a Schrödinger-like equation with the perturbation* (101)*. Both forms represent the complete interaction between the particles and are exactly equivalent to the original Bethe-Salpeter equation* (42)*.*

The main difference between the original form of the BS equation and the Schrödinger-like form derived here is primarily that the latter has the time dependence reduced to a single time, which makes the wave function in accord with standard quantum mechanics. Furthermore, the Schrödinger-like form contains explicitly the resolvent, while the remaining part of the Green's function (145) is merged with the kernel κ to form the potential $\mathcal{V}$.

The Schrödinger-like equation (113) we have derived is equivalent to the equation derived from the BS equation by Sucher [38, Eq. 1.47] and rederived by Douglas and Kroll [40, Eq. 3.26] and Zhang [43, Eq. 15]. In these works the equation is essentially obtained by integrating over the relative energy of the particles, thereby transforming the equation to an "equal-time" equation. This equation is then analyzed in terms of the Brillouin-Wigner perturbation theory. In our presentation the corresponding equation is obtained by starting from MBPT in the Rayleigh-Schrödinger formulation and summing all relevant perturbations to all orders. The present derivation therefore can serve as a link between the two approaches.

In the next section we shall extend the treatment to the quasi-degenerate case and derive the corresponding Bloch equation.

5.3. Derivation of the Bethe-Salpeter-Bloch equation. Quasi-degenerate model space.

We have previously assumed that the model space is *degenerate*, which for a two-electron system implies that the effective interaction is *diagonal* within this space (assuming the basis functions have definite symmetry). Then the relation (104) simplifies the treatment, and the formulas derived in the previous section lead directly to the standard Bethe-Salpeter equation (113). The treatment above, however, is more general and can be extended to the case where the model space is non-degenerate (quasi-degenerate). In the present section we shall show how this can be performed.

The following relation can easily derived by induction, when operating to the right on the model space,

$$\frac{\partial^n \bar{\Omega}}{\partial \mathcal{E}^n} = \Gamma_Q \frac{\partial^n (\mathcal{V}\bar{\Omega})}{\partial \mathcal{E}^n} - n\Gamma_Q \frac{\partial^{(n-1)} \bar{\Omega}}{\partial \mathcal{E}^{(n-1)}} \tag{114}$$

To prove this we form the next-order derivative

$$\frac{\partial^{(n+1)} \bar{\Omega}}{\partial \mathcal{E}^{(n+1)}} = -\Gamma_Q^2 \frac{\partial^n (\mathcal{V}\bar{\Omega})}{\partial \mathcal{E}^n} + \Gamma_Q \frac{\partial^{(n+1)} (\mathcal{V}\bar{\Omega})}{\partial \mathcal{E}^{(n+1)}} + n\Gamma_Q^2 \frac{\partial^{(n-1)} \bar{\Omega}}{\partial \mathcal{E}^{(n-1)}} - n\Gamma_Q \frac{\partial^n \bar{\Omega}}{\partial \mathcal{E}^n}$$

(Since no singularities are involved here, ordinary rules of derivation can be used.) Inserting the expression (114) in the first term, yields

$$\frac{\partial^{(n+1)} \bar{\Omega}}{\partial \mathcal{E}^{(n+1)}} = \Gamma_Q \frac{\partial^{(n+1)} (\mathcal{V}\bar{\Omega})}{\partial \mathcal{E}^{(n+1)}} - (n+1)\Gamma_Q \frac{\partial^n \bar{\Omega}}{\partial \mathcal{E}^n}$$

From the identity $\bar{\Omega} = 1 + \Gamma_Q \mathcal{V}\bar{\Omega}$ we obtain the first derivative (operating on P)

$$\frac{\partial \bar{\Omega}}{\partial \mathcal{E}} = \Gamma_Q \frac{\partial (\mathcal{V}\bar{\Omega})}{\partial \mathcal{E}} - \Gamma_Q \bar{\Omega}$$

which completes the proof of the relation (114).

The formula above leads together with the expansion (100) to

$$Q\Omega P = Q\bar{\Omega}P + \Gamma_Q \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n (\mathcal{V}\bar{\Omega})}{\partial \mathcal{E}^n} (H'_{\text{eff}})^n - \Gamma_Q \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \frac{\partial^{(n-1)} \bar{\Omega}}{\partial \mathcal{E}^{(n-1)}} (H'_{\text{eff}})^n \tag{115}$$

The first term on the rhs can also be expressed $\Gamma_Q \mathcal{V}\bar{\Omega}P$, and the last term is simply $-\Gamma_Q \Omega H'_{\text{eff}}$, which yields

$$Q\Omega P = \Gamma_Q \Big[\mathcal{V}\bar{\Omega}P + \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n (\mathcal{V}\bar{\Omega})}{\partial \mathcal{E}^n} (H'_{\text{eff}})^n - \Omega H'_{\text{eff}} \Big] \tag{116}$$

We can consider $\mathcal{V}\bar{\Omega}$ as a single energy-dependent operator, and if that operates on a particular model state of a degenerate model space of energy E_0, the first two terms of the bracket above represents the Taylor expansion

$$\mathcal{V}(E_0)\,\bar{\Omega}(E_0) + \sum_{n=1}^{\infty} \frac{1}{n!}\,\frac{\partial^n(\mathcal{V}\bar{\Omega})}{\partial\mathcal{E}^n}\Big|_{E_0}\,(\Delta E^\alpha)^n = \mathcal{V}(E^\alpha)\,\bar{\Omega}(E^\alpha). \tag{117}$$

Thus, the expansion has the effect of transforming the energy parameter of the product $\mathcal{V}\bar{\Omega}$ from E_0 to the full energy E^α,

$$\mathcal{V}(E_0)\bar{\Omega}(E_0)|\Psi_0^\alpha\rangle \to \mathcal{V}(E^\alpha)\bar{\Omega}(E^\alpha)|\Psi_0^\alpha\rangle \tag{118}$$

in analogy with the expansion (106). Using the relation (107), the equation (116) above then becomes

$$Q\Omega|\Psi_0^\alpha\rangle = \Gamma_Q\big[\mathcal{V}(E^\alpha)\Omega - \Omega H'_{\rm eff}\big]|\Psi_0^\alpha\rangle \tag{119}$$

or

$$(E_0 - H_0)\Omega|\Psi_0^\alpha\rangle = Q\big[\mathcal{V}(E^\alpha)\Omega - \Omega H'_{\rm eff}\big]|\Psi_0^\alpha\rangle \tag{120}$$

which is consistent with the Bethe-Salpeter equation (113).

If the model space is *non-degenerate* (quasi-degenerate), then the relation (104) is no longer valid, and the expansion (116) can not be expressed by means of a single energy parameter as in the Taylor expansion (117). Instead, the potential will depend on the *full matrix* of the effective Hamiltonian. We then replace the energy parameter in (103) by the model Hamiltonian H_0,

$$\bar{\Omega}P = P + \Gamma_Q(H_0)\mathcal{V}(H_0) + \cdots = \bar{\Omega}(H_0)P$$

By this notation we understand—in accordance with the rule (102)—

$$A(H_0)B|\Phi\rangle = A(E_0)B|\Phi\rangle \tag{121}$$

when $|\Phi\rangle$ represents an eigenstate of H_0 with the eigenvalue E_0 and B is an arbitrary operator combination. Together with the linearity condition,

$$A(H_0)B\big|a\Phi + b\Phi'\big\rangle = aA(E_0)B|\Phi\rangle + bA(E'_0)B|\Phi'\rangle \tag{122}$$

where $|\Phi'\rangle$ represents another eigenstate of H_0 with the eigenvalue E'_0, this defines the notation fully.

The expansion (116) can now be regarded, in analogy with the energy modification (117), as modifying the parameter H_0 to the full effective Hamiltonian $H_{\rm eff} = H_0 + H'_{\rm eff}$

$$\mathcal{V}(H_0)\,\bar{\Omega}(H_0) + \sum_{n=1}^{\infty} \frac{1}{n!}\,\frac{\partial^n(\mathcal{V}\bar{\Omega})}{\partial\mathcal{E}^n}\,(H'_{\rm eff})^n = \mathcal{V}(H_{\rm eff})\,\bar{\Omega}(H_{\rm eff}) \tag{123}$$

i.e.,

$$\mathcal{V}(H_0)\bar{\Omega}(H_0)P \to \mathcal{V}(H_{\rm eff})\bar{\Omega}(H_{\rm eff})P \tag{124}$$

and Eq. (119) becomes

$$Q\Omega P = \Gamma_Q(H_0)\mathcal{V}(H_{\rm eff})\bar{\Omega}(H_{\rm eff})P - \Gamma_Q(H_0)\Omega H'_{\rm eff} \tag{125}$$

The notation here is defined by the relation

$$A(H_{\rm eff})B|\Psi_0^\alpha\rangle = A(E^\alpha)B|\Psi_0^\alpha\rangle \tag{126}$$

where $|\Psi_0^\alpha\rangle$ represents a model state (eigenstate of $H_{\rm eff}$ with the eigenvalue E^α, see Eq. 17), which together with the linearity condition defines the operator when acting on any model space.

Similarly, the expansion (100) yields

$$\Omega P = \bar{\Omega}(H_0)P + \sum_{n=1}^{\infty} \frac{1}{n!}\,\frac{\partial^n \bar{\Omega}}{\partial \mathcal{E}^n}\,\left(H'_{\rm eff}\right)^n = \bar{\Omega}(H_{\rm eff})P \tag{127}$$

and we can now express the equation (125) as

$$Q\Omega P = \Gamma_Q(H_0)\mathcal{V}(H_{\rm eff})\,\Omega P - \Gamma_Q(H_0)\Omega\, H'_{\rm eff} \tag{128}$$

or

$$\big[\Gamma_Q(H_0)\big]^{-1} Q\Omega P = Q\big[\mathcal{V}(H_{\rm eff})\,\Omega - \Omega\, H'_{\rm eff}\big]P \tag{129}$$

We now apply the definition (121) above with $A(\mathcal{E}) = \big[\Gamma_Q(\mathcal{E})\big]^{-1} = Q(\mathcal{E} - H_0)$. Then, with $|\Phi(E_0)\rangle$ being an eigenvector of H_0 with the eigenvalue E_0, we have

$$A(E_0)\,Q\Omega\big|\Phi(E_0)\big\rangle = (E_0 - H_0)\,\Omega\big|\Phi(E_0)\big\rangle = \big[\Omega, H_0)\big]\big|\Phi(E_0)\big\rangle$$

Therefore, *the inverse of the resolvent can be expressed as a commutator*

$$\big[\Gamma_Q(H_0)\big]^{-1} Q\Omega P \equiv [\Omega, H_0]P \tag{130}$$

which leads to the commutator relation

$$[\Omega, H_0]P = Q\big[\mathcal{V}(H_{\rm eff})\,\Omega - \Omega\, H'_{\rm eff}\big]P \tag{131}$$

The relation (112) can be generalized to

$$H'_{\rm eff} = P\mathcal{V}(H_{\rm eff})\,\Omega P \tag{132}$$

and with the IN relation (67) $P\Omega P = P$ we arrive at *the BS equation in commutator form*

$$\boxed{\big[\Omega, H_0\big]P = \mathcal{V}(H_{\rm eff})\,\Omega P - \Omega\, H'_{\rm eff}} \tag{133}$$

We refer to this equation as the ***Bethe-Salpeter-Bloch equation****, and it represents the main result of the present work. It is a multi-state equation in contrast to the standard BS equation* (113) *that is state specific. The BS-Bloch equation has the same relation to the standard BS equation as has the standard Bloch equation* (19a) *to the ordinary Schrödinger equation.* The dependence on the effective Hamiltonian makes it a *matrix-operator equation* and therefore somewhat more complicated to solve than the standard Bloch equation. Below we shall indicate how also this equation can be solved perturbatively.

5.4. Perturbative expansion of the Bethe-Salpeter-Bloch equation

We consider now the perturbative expansion of the BS-Bloch equation with a sequence of separable single-photon exchange (potential V), as illustrated in Fig: 7. In first order the BS-Bloch equation becomes

$$\big[\Omega^{(1)}, H_0\big]|ab\rangle = QV(H_{\rm eff})|ab\rangle \tag{134}$$

and here the argument $H_{\rm eff}$ of the potential is approximated by H_0. In the next order we have

$$\big[\Omega^{(2)}, H_0\big]|ab\rangle = QV(H_{\rm eff})\,\Omega^{(1)}|ab\rangle - \Omega^{(1)}|cd\rangle\langle cd|H^{(1)}_{\rm eff}|ab\rangle \tag{135}$$

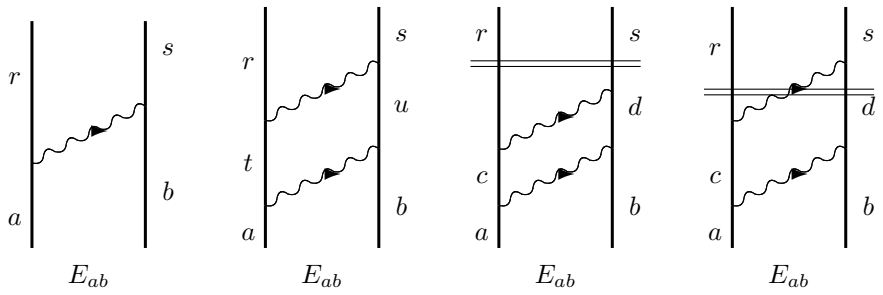

Fig. 7. Exchange of one- and two-photon ladder, starting from the model-space state $|ab\rangle$ of energy E_{ab} (a,b). The diagram (c) is a standard "*folded*" diagram with a double denominator, indicated by the double horizontal line. Diagram (d) is the folded diagram with wave function with uncontracted photon, described in the next section.

and here $H_{\rm eff}$ is approximated by $H_0 + H^{(1)}_{\rm eff}$. The last term is the *folded* diagram, with summation over the model-space states $|cd\rangle$ and represented by the diagram (c) in Fig. 7. The contribution to the wave-operator matrix element $\langle rs|\Omega^{(2)}|cd\rangle$ becomes

$$-\frac{\langle rs|\Omega^{(1)}|cd\rangle}{(E_{ab}-E_{rs})}\,\langle cd|H^{(1)}_{\rm eff}|ab\rangle = -\frac{\langle rs|V|cd\rangle\langle cd|V|ab\rangle}{(E_{ab}-E_{rs})(E_{cd}-E_{rs})} \tag{136}$$

with $E_{xy} = \varepsilon_x + \varepsilon_y$. This represents the part of the model-space contribution (MSC) (182) that is due to the variation of the resolvent

$$\frac{\delta}{\delta\mathcal{E}}\,\Gamma_Q \Rightarrow -\frac{1}{(E_{ab}-E_{rs})(E_{cd}-E_{rs})}$$

with the potential unchanged. The remaining part of the MSC, due to the potential variation, is taken care of by modifying the parameter of the potential in $V(H_{\rm eff})$. The latter is a *matrix operator*, implying that the resulting second-order wave operator will also be in the form of a matrix operator [3].

In practice, the equation is solved *iteratively* (se Eq. 19d), which implies that also the parameter of the potential is successively updated. By continuing this process, a perturbation expansion of the Bethe-Salpeter-Bloch equation is generated. This is a *multi-state* expansion, valid for the entire model space. This is in contrast to the *state-specific* Brillouin-Wigner expansion (106) of the ordinary BS equation (113).

As usual, of course, nothing can generally be said about the convergence condition. In a multi-state expansion it is expected that so-called *intruder states* may cause convergence difficulties, as with the ordinary Bloch equation. One way to remedy the situation could be to employ the *intermediate Hamiltonian approach*, successfully applied in several standard MBPT calculations [74, 75, 76, 77]. There should be no principal difficulty in applying this formalism to the Bethe-Salpeter-Bloch equation.

In the next section we shall describe a new procedure for solving the BS-Bloch equation, which automatically yields the correct model-space contributions, including those due to the energy-dependence of the interaction.

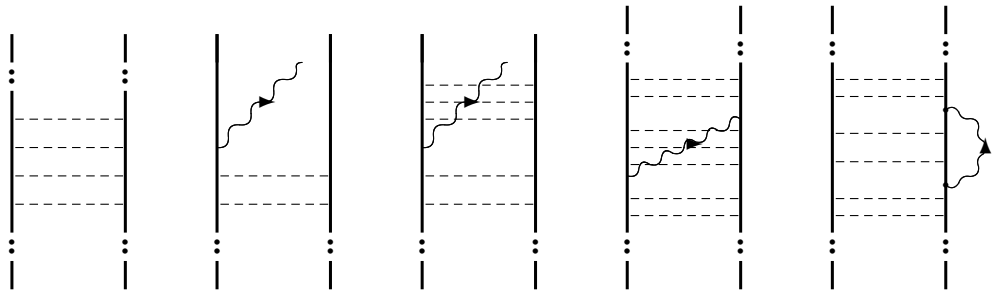

Fig. 8. Illustration of the new perturbative procedure for solving the Bethe-Salpeter equation, described in the text. The horizontal dotted lines represent instantaneous Coulomb(-Breit) interactions and the wavy lines fully covariant photons.

5.5. New numerical procedure for solving the Bethe-Salpeter-Bloch equation

We shall here briefly describe the numerical procedure we have developed for solving the BS-Bloch equation [64, Sect. 8]. A more detailed account of the procedure together with numerical results will appear in a separate publication [78].

The procedure is a combination of perturbative (order-by-order) and non-perturbative ("all-order") techniques, and the starting point is the iterative solution of relativistic pair equations [79, 80, 81, 82, 47] with instantaneous Coulomb (or Coulomb/Breit) interactions. This represents the (all-order) "ladder" approximation of the BS equation, as indicated in Fig. 8 (a). The pair function is then combined with the emission of a single (uncontracted) photon (Fig. 8 b), which leads to a new pair function for each value of the photon momentum k. This represents a wave function lying in the extended Fock space, discussed in section 4.3. The photon is subsequently annihilated on the same or the other electron, and integration over the photon momentum yields the complete single-photon exchange. Before the annihilation, the pair function can be iterated further (Fig. 8 c), which yields instantaneous Coulomb (-Breit) interactions, crossing the photon. The iterations can be continued also after the annihilation, as indicated in Fig. 8 (d). Annihilating the photon on the same electron line, leads to the radiative self-energy and vertex corrections (Fig. 8 e), which, of course, have to be properly renormalized.

In the procedure described here, the QED effects are evaluated by means of *correlated* wave functions, in contrast to the conventional S-matrix procedure, where uncorrelated products of hydrogenic orbitals are used [61]. Therefore, this numerical technique will be comparable to the analytical "unified model" of Drake and coworkers [45, 46]. Our method can hardly match the latter in numerical accuracy but will instead contain many effects not included in the analytical approach. Therefore, a *combination* of the two approaches might lead to the best result.

For computational reasons it is at present not possible to treat more than one covariant photon with our new procedure (although there is no principal limit). However, even with a single covariant photon, the dominating part of the multi-photon exchange will be included, due to the crossings with the instantaneous interactions (Fig. 8 c). Also single and double *virtual electron-positron pairs* can be included in the intermediate states. Therefore, this procedure will, for instance, correspond to all effects treated by Zhang [44] in his analysis of the helium fine structure up to order $m\alpha^7$, except for the non-separable interaction of two retarded photons (Fig. 6), for which we have at present to use the

[3] The concept of a *matrix operator* should not be confused with the matrix representation of an ordinary quantum-mechanical operator. A matrix operator is a matrix where each element is a distinct operator.

analytical approximation.

We shall now indicate that the procedure described here automatically leads to the correct model-space contributions, including the contribution due to the modification of the potential. For that purpose we return to the situation discussed above in Fig. 7. In the new procedure there will also be a folded diagram associated with the wave function with an *uncontracted* photon. This gives rise to the diagram in Fig. 7 (d) with a double denominator *inside* the potential. Generally, the emission of a photon in the *forward* direction corresponds according to the relation (165) to the expression

$$\langle rs|V(\mathcal{E})|tu\rangle = \Big\langle rs\Big| \int \mathrm{d}k\, f(k) \frac{1}{\mathcal{E} - E_{ru} - k}\Big|tu\Big\rangle \tag{137}$$

if particle states are involved. The folded diagram with an uncontracted photon gives after absorbing the photon in analogy with the ordinary folds rise to the contribution

$$-\Big\langle rs\Big| \int \mathrm{d}k\, f(k) \frac{1}{(E_{ab} - E_{rd} - k)(E_{cd} - E_{rd} - k)}\Big|cd\Big\rangle \tag{138}$$

which corresponds to the difference ratio

$$\frac{\delta V(\mathcal{E})}{\delta \mathcal{E}}$$

Therefore, this contribution takes care of the potential modification and together with the ordinary folded diagram (136) represents the entire MSC in the second-order wave operator.

6. Summary and conclusions

Standard many-body perturbation theory (MBPT) is conveniently based upon the Bloch equation, which is the generating equation for the Rayleigh-Schrödinger perturbation expansion. The Bloch equation can also be used to generate various other perturbative schemes, such as the linked-diagram expansion, and it also leads to non-perturbative (all-order) schemes, such as the Coupled-Cluster Approach. In the commutator form (19a) the Bloch equation leads to schemes that can handle the quasi-degenerate problem in an efficient way by means of an ”extended” model space.

In this paper we have reviewed the connection between relativistic MBPT and quantum-electrodynamics (QED) for a two-electron system by means of the recently introduced covariant-evolution-operator method [64]. The exchange of a single covariant photon is treated to all orders, and this is shown to lead to an equation of the Bethe-Salpeter (BS) type. Extending the treatment to all non-separable interactions (including radiative corrections) leads to the full BS equation. This establishes a link between the perturbative schemes, based upon Rayleigh-Schrödinger perturbation theory and schemes based upon the BS equation, which are normally treated by means of the Brillouin-Wigner perturbation procedure.

In addition, a Bloch equation in commutator form that is compatible with the BS equation is derived. This equation is a multi-state equation, valid for the entire model space—in contrast to the standard BS equation that is state specific. The BS-Bloch equation has the same relation to the Bethe-Salpeter equation as has the standard Bloch equation to the ordinary Schrödinger equation and represents a series of BS equations, associated with a model space that need not be degenerate.

It is demonstrated that a multi-state perturbative expansion of the BS-Bloch equation can be generated, quite similar to the standard MBPT expansions. In principle, this will make it possible to treat the quasi-degeneracy problem perturbatively also within the BS formalism. Such a scheme is presently being tested at our laboratory.

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APPENDIX

A. Zeroth-order Green's function

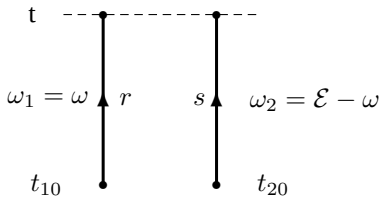

Fig. 9. Graphical representation of the zeroth-order Green's function (139).

The zeroth-order Green's function (36) in Fig. 9 is in coordinate representation

$$G_0(x_1x_2; x_{10}x_{20}) = S_{\rm F}(x_1; x_{10})\, S_{\rm F}(x_2; x_{20}) \tag{139}$$

where $S_{\rm F}$ is the electron propagator

$$S(x, x_0) = \int \frac{{\rm d}\omega}{2\pi}\, S(\omega)\, {\rm e}^{-{\rm i}\omega(t-t_0)} \tag{140}$$

with the fourier transform

$$\langle \boldsymbol{x}|S(\omega)|\boldsymbol{x}_0\rangle = \frac{\langle \boldsymbol{x}|r\rangle\langle r|\boldsymbol{x}_0\rangle}{\omega - \varepsilon_r + {\rm i}\eta_r} = \langle \boldsymbol{x}|\hat{S}(\omega)|\boldsymbol{x}_0\rangle \tag{141}$$

and the corresponding operator form

$$\hat{S}(\omega) = \frac{\Lambda_+}{\omega - h + {\rm i}\eta} + \frac{\Lambda_-}{\omega - h - {\rm i}\eta} \tag{142}$$

Here, h is the single-electron Dirac Hamiltonian in the field of the nucleus and $\Lambda_\pm$ are projection operators for positive and negative-energy single-particle states.

We consider the equal-times Green's function with $t_1 = t_2 = t$, which gives

$$\begin{aligned} G_0(t, \boldsymbol{x}_1, \boldsymbol{x}_2; x_{10}, x_{20}) &= \int \frac{{\rm d}\epsilon}{2\pi}\, {\rm e}^{-{\rm i}\epsilon t}\, \frac{\langle \boldsymbol{x}_1\boldsymbol{x}_2|rs\rangle\langle rs|\boldsymbol{x}_{10}\boldsymbol{x}_{20}\rangle}{\epsilon - \varepsilon_r - \varepsilon_s} \\ \times \quad \int \frac{{\rm d}\omega}{2\pi} \Big[\frac{1}{\omega - \varepsilon_r + {\rm i}\eta_r} &+ \frac{1}{\epsilon - \omega - \varepsilon_s + {\rm i}\eta_s}\Big]\, {\rm e}^{{\rm i}\omega t_{10}}\, {\rm e}^{{\rm i}(\epsilon-\omega)t_{20}} \end{aligned} \tag{143}$$

with $x = (t, \boldsymbol{x})$, $\omega_1 = \omega$ and $\epsilon = \omega_1 + \omega_2$. The fourier transform with respect to t is then

$$\begin{aligned} &G_0(\epsilon, \boldsymbol{x}_1, \boldsymbol{x}_2; x_{10}, x_{20}) = \\ &\frac{\langle \boldsymbol{x}_1\boldsymbol{x}_2|rs\rangle\langle rs|\boldsymbol{x}_{10}\boldsymbol{x}_{20}\rangle}{\epsilon - \varepsilon_r - \varepsilon_s} \int \frac{{\rm d}\omega}{2\pi} \Big[\frac{1}{\omega - \varepsilon_r + {\rm i}\eta_r} + \frac{1}{\epsilon - \omega - \varepsilon_s + {\rm i}\eta_s}\Big]\, {\rm e}^{{\rm i}\omega t_{10}}\, {\rm e}^{{\rm i}(\epsilon-\omega)t_{20}} \end{aligned} \tag{144}$$

or in operator form

$$G_0(\epsilon) = \Gamma(\epsilon) \int \frac{\mathrm{d}\omega}{2\pi}\, g_0(\epsilon,\omega)\, \mathrm{e}^{\mathrm{i}\omega t_{10}}\, \mathrm{e}^{\mathrm{i}(\epsilon-\omega)t_{20}} \tag{145}$$

where $\Gamma(\mathcal{E})$ is the resolvent (4)

$$\Gamma(\mathcal{E}) = \frac{1}{\mathcal{E} - H_0} \tag{146}$$

$H_0 = h_1 + h_2$ is the zeroth-order Hamiltonian (30) and

$$\begin{aligned} g_0(\epsilon,\omega) &= \Lambda_+\Big[\frac{1}{\omega - h_1 + \mathrm{i}\eta} + \frac{1}{\epsilon - \omega - h_2 + \mathrm{i}\eta}\Big] \\ &+ \Lambda_-\Big[\frac{1}{\omega - h_1 - \mathrm{i}\eta} + \frac{1}{\epsilon - \omega - h_2 - \mathrm{i}\eta}\Big] \end{aligned} \tag{147}$$

The inverse transformation is

$$\boxed{G_0(t, \boldsymbol{x}_1, \boldsymbol{x}_2; x_{10}, x_{20}) = \int \frac{\mathrm{d}\epsilon}{2\pi}\, \mathrm{e}^{-\mathrm{i}\epsilon t}\, G_0(\epsilon, \boldsymbol{x}_1, \boldsymbol{x}_2; x_{10}, x_{20})} \tag{148}$$

and specifically,

$$\boxed{G_0(t=0, \boldsymbol{x}_1, \boldsymbol{x}_2; x_{10}, x_{20}) = \int \frac{\mathrm{d}\epsilon}{2\pi}\, G_0(\epsilon, \boldsymbol{x}_1, \boldsymbol{x}_2; x_{10}, x_{20})} \tag{149}$$

B. Single-photon exchange

(See Ref. [64, Eq. 312 and App. A1].)
We consider now the covariant evolution operator (49) for the exchange of a single covariant photon, represented by the diagram in Fig. 10 (left)

$$\begin{aligned} U^{(1)}(t', t_0) &= -\frac{1}{2} \iint \mathrm{d}^3\boldsymbol{x}_1'\, \mathrm{d}^3\boldsymbol{x}_2'\, \hat{\psi}^\dagger(x_1')\hat{\psi}^\dagger(x_2') \iint \mathrm{d}^4x_1\, \mathrm{d}^4x_2\, \mathrm{i}S_\mathrm{F}(x_1', x_1)\, \mathrm{i}S_\mathrm{F}(x_2', x_2)\, \mathrm{i}I(x_2, x_1) \\ &\times \iint \mathrm{d}^3\boldsymbol{x}_{10}\, \mathrm{d}^3\boldsymbol{x}_{20}\, \mathrm{i}S_\mathrm{F}(x_1, x_{10})\, \mathrm{i}S_\mathrm{F}(x_2, x_{20})\, \hat{\psi}(x_{20})\hat{\psi}(x_{10}) \end{aligned} \tag{150}$$

leaving out the damping factors. More compactly, we express this as

$$\begin{aligned} U^{(1)}(t', t_0) &= -\frac{1}{2}\hat{\psi}^\dagger(x_1')\hat{\psi}^\dagger(x_2')\, G_0(x_1', x_2'; x_1 x_2)\, \mathrm{i}I(x_2, x_1) \\ &\times G_0(x_1, x_2; x_{10} x_{20})\, \hat{\psi}(x_{20})\hat{\psi}(x_{10}) \end{aligned} \tag{151}$$

with integrations over all variables that do not appear on the left-hand side. Here, $I(x_2, x_1)$ represents the single-photon exchange

$$I(x_2, x_1) = e\alpha_1^\mu D_{\mathrm{F}\mu\nu}(x_2 - x_1)\, e\alpha_2^\nu = \int \frac{\mathrm{d}z}{2\pi}\, \mathrm{e}^{-\mathrm{i}z(t_2 - t_1)}\, I(z, \boldsymbol{x}_2, \boldsymbol{x}_1) \tag{152}$$

where $D_{\mathrm{F}\mu\nu}(x_2 - x_1)$ is the *Feynman photon propagator*. The electron-field operator is in the interaction picture [31]

$$\hat{\psi}(x) = \hat{\psi}(t, \boldsymbol{x}) = c_j \phi_j(\boldsymbol{x})\, \mathrm{e}^{-\mathrm{i}\varepsilon_j t} \tag{153}$$

where ϕ_j are eigenfunctions of the single-electron Hamiltonian in the nuclear field (Furry picture)

$$h_0\, \phi_j(\boldsymbol{x}) = \varepsilon_j \phi_j(\boldsymbol{x}) \tag{154}$$

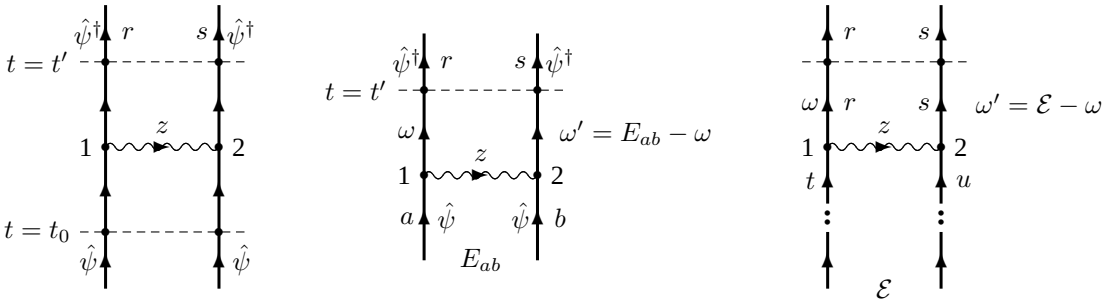

Fig. 10. Graphical representation of the covariant-evolution operator for single-photon exchange in the form (150) (left) and in the form (155) with $t_0 \to -\infty$.

If we operate with the expression (151) to the right on a *positive-energy state*, we can use the relations (51) to simplify the expression. Furthermore, since in that case $t_0 \le t_1, t_2$ and since t_1, t_2 run from $-\infty$ to $+\infty$, we must have $t_0 = -\infty$, yielding

$$U^{(1)}(t', -\infty) = \frac{1}{2}\hat\psi^\dagger(x_1')\hat\psi^\dagger(x_2')\, G_0(x_1', x_2'; x_1 x_2)\, \mathrm{i}I(x_2, x_1)\ \hat\psi(x_2)\hat\psi(x_1) \tag{155}$$

We shall always assume that we operate to the right on an unperturbed state, which with the adiabatic damping (29) corresponds to $t_0 = -\infty$. Therefore, we shall in the following normally suppress this argument.

We now use the form of the Green's function derived in the previous Appendix

$$G_0(x_1', x_2'; x_1, x_2) = \int \frac{\mathrm{d}\epsilon}{2\pi}\, \mathrm{e}^{-\mathrm{i}\epsilon t'}\, G_0(\epsilon) = \int \frac{\mathrm{d}\epsilon}{2\pi}\, \mathrm{e}^{-\mathrm{i}\epsilon t'}\, \Gamma(\epsilon) \int \frac{\mathrm{d}\omega}{2\pi}\, g_0(\epsilon, \omega)\, \mathrm{e}^{\mathrm{i}\omega t_1}\, \mathrm{e}^{\mathrm{i}(\epsilon-\omega)t_2} \tag{156}$$

to evaluate the matrix element of the evolution operator (see Fig. 10, middle), which yields (leaving out the time integrations)

$$\begin{aligned} & U^{(1)}(t')\,\big|ab\big\rangle = \big\langle rs\big| \int \frac{\mathrm{d}\epsilon}{2\pi}\, \Gamma(\epsilon)\, \mathrm{e}^{-\mathrm{i}t'(\epsilon - E_{rs}} \\ \times\ & \int \frac{\mathrm{d}\omega}{2\pi}\, g_0(\epsilon, \omega) \int \frac{\mathrm{d}z}{2\pi}\, \mathrm{i}I(z) \mathrm{e}^{-\mathrm{i}t_1(\varepsilon_a - z - \omega)}\, \mathrm{e}^{-\mathrm{i}t_2(\varepsilon_b + z - \epsilon + \omega)}\, \big|ab\big\rangle \end{aligned} \tag{157}$$

Here, $|ab\rangle$ and $|rs\rangle$ represent straight product states (non-antisymmetrized, which eliminates the factor of $\frac{1}{2}$) of energy $E_{ab} = \varepsilon_a + \varepsilon_b$ and $E_{rs} = \varepsilon_r + \varepsilon_s$, respectively . After integrations this becomes

$$\begin{aligned} & \big\langle rs\big|U^{(1)}(t')\,\big|ab\big\rangle = \big\langle rs\big| \int \frac{\mathrm{d}\epsilon}{2\pi}\, \mathrm{e}^{-\mathrm{i}t'(\epsilon - E_{rs})} \Gamma(\epsilon) \int \frac{\mathrm{d}\omega}{2\pi}\, g_0(\epsilon, \omega) \int \frac{\mathrm{d}z}{2\pi}\, \mathrm{i}I(z) \\ \times\ & 2\pi\delta(\varepsilon_a - z - \omega)\, 2\pi\delta(\varepsilon_a + \varepsilon_b - \epsilon)\big|ab\big\rangle \\ =\ & \big\langle rs\big|\mathrm{e}^{-\mathrm{i}t'(E_{ab} - \varepsilon_r - \varepsilon_s)} \Gamma(E_{ab}) \int \frac{\mathrm{d}\omega}{2\pi}\, g_0(E_{ab}, \omega)\, \mathrm{i}I(\varepsilon_a - \omega)\big|ab\big\rangle \end{aligned} \tag{158}$$

We can also express this result as

$$U^{(1)}(t)\big|ab\big\rangle = \mathrm{e}^{-\mathrm{i}t(E_{ab} - H_0)}\, \Gamma(E_{ab})\, V(E_{ab})\, \big|ab\big\rangle \tag{159}$$

where

$$V(E_{ab}) = \int \frac{\mathrm{d}\omega}{2\pi}\, g_0(E_{ab}, \omega)\, \mathrm{i}I(\varepsilon_a - \omega) \tag{160}$$

The results above can be generalized to the case where we operate to the right on a state of a general energy $\mathcal{E}$ (see Fig. 10 right)

$$U^{(1)}(t)\,F(\mathcal{E}) = \mathrm{e}^{-\mathrm{i}t(\mathcal{E}-H_0)}\,\Gamma(\mathcal{E})V(\mathcal{E})\,F(\mathcal{E}) \tag{161}$$

The corresponding wave operator, using the definition (66), is

$$\boxed{\Omega^{(1)}(\mathcal{E}) = Q\widetilde{U}^{(1)}(0) = \Gamma_Q(\mathcal{E})V(\mathcal{E})} \tag{162}$$

where

$$\Gamma_Q(\mathcal{E}) = Q\Gamma(\mathcal{E}) = \frac{Q}{\mathcal{E}-H_0} \tag{163}$$

The effective interaction is obtained from the relation (68) by taking the time derivative at $t = 0$, which eliminates the resolvent,

$$\boxed{H^{(1)}_{\mathrm{eff}}(\mathcal{E}) = PV(\mathcal{E})\,P} \tag{164}$$

With the explicit form of the interaction (152) the matrix elements of the potential for the exchange of a single covariant photon becomes in the *Feynman gauge* [64, App. A]

$$\langle rs|V(\mathcal{E})|tu\rangle = \Big\langle rs\Big|\int \mathrm{d}k\, f(k)\Big[\frac{1}{\mathcal{E}-\varepsilon_r-\varepsilon_u-(k-\mathrm{i}\gamma)_r}+\frac{1}{\mathcal{E}-\varepsilon_s-\varepsilon_t-(k-\mathrm{i}\gamma)_s}\Big]\Big|tu\Big\rangle \tag{165}$$

where the $A_r = A\,\mathrm{sgn}(\varepsilon_r)$, and the function $f(k)$ is given by

$$f(k) = -\frac{e^2}{4\pi^2}\,(1-\boldsymbol{\alpha_1}\cdot\boldsymbol{\alpha_2})\,\frac{\sin(kr_{12})}{r_{12}} \tag{166}$$

The last factor can be expanded as

$$\frac{\sin(kr_{12})}{r_{12}} = k\sum_{l=0}^{\infty}(2l+1)j_l(kr_1)j_l(kr_2)\,\boldsymbol{C}^{(l)}(1)\cdot\boldsymbol{C}^{(l)}(2) \tag{167}$$

where j_l are spherical Bessel functions and $\boldsymbol{C}^{(l)}$ spherical tensors, closely related to the spherical harmonics.

In the *Coulomb gauge* the potential can be separated into an instantaneous and an retarded part,

$$V(\mathcal{E}) = V_{\mathrm{I}} + V_{\mathrm{R}}(\mathcal{E})$$

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

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

and the retarded part is given by the same expression as in the Feynman gauge (165) with

$$f(k) = \frac{e^2}{4\pi^2}\Big[-\boldsymbol{\alpha_1}\cdot\boldsymbol{\alpha_2}\frac{\sin(kr_{12})}{r_{12}} + (\boldsymbol{\alpha_1}\cdot\boldsymbol{\nabla_1})\,(\boldsymbol{\alpha_2}\cdot\boldsymbol{\nabla_2})\frac{\sin(kr_{12})}{k^2\,r_{12}}\Big] \tag{168}$$

where the nabla operators do not operate beyond the square bracket.

C. Separable two-photon exchange

(See Ref. [64, Sect.5.2.1 and App.A.2])
Next we consider the separable two-photon exchange for which there is an intermediate time ($t = t''$) with no free or uncontracted photons, as illustrated in Fig. 11 (left). Operating to the far right on a state of the energy $\mathcal{E}$, the evolution operator can in analogy with the single-photon exchange (161) be expressed

$$U^{(2)}(t) = \mathrm{e}^{-\mathrm{i}t(\mathcal{E}-H_0)}\,\Gamma V \Gamma V = \mathrm{e}^{-\mathrm{i}t(\mathcal{E}-H_0)}\,U^{(1)}(0)\,U^{(1)}(0) \tag{169}$$

where $\Gamma = \Gamma(\mathcal{E})$ is the resolvent (146) and $V = V(\mathcal{E})$ is the single-photon potential (160). Here, the intermediate states run over *all* states — in the Q as well as the P space — and when the intermediate state lies in the model space (P), *(quasi)singularities* may occur. These singularities are removed in the *reduced evolution operator* (54) by the *counterterms* (56)

$$\widetilde{U}(t)P = U(t)P + C(t) \tag{170}$$

The counterterm is in the present case given by the product of two single-photon contributions, as

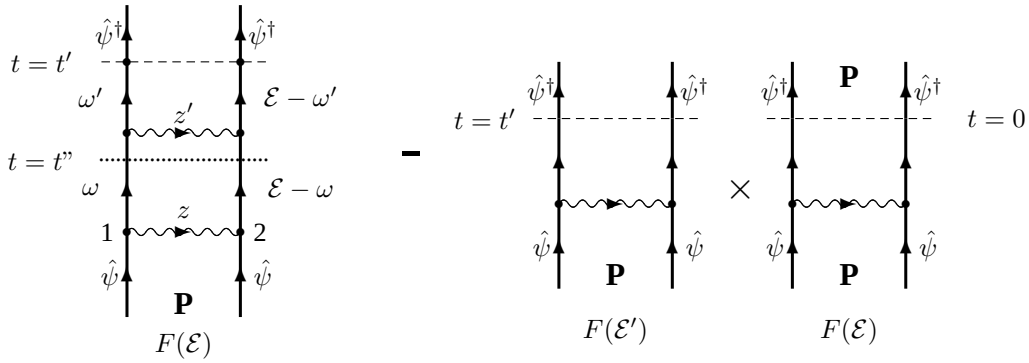

Fig. 11. Graphical representation of the separable two-photon-photon ladder diagram (left). This diagram is separable, if there exists a time (represented by the dotted line) at which there is no uncontracted photon, i.e., a time after the first photon has been absorbed and before the second has been created. The corresponding counterterm (right) is a product of two operators, which evolve independently from possibly different states of the model space.

shown in Fig. 11 (right)

$$C^{(2)}(t) = -U^{(1)}(t)P \cdot PU^{(1)}(0)P \tag{171}$$

The two factors evolve independently from (possibly different) states in the model space, which is indicated by the "dot". The counterterm eliminates the singularity, but there may be a *finite remainder*, which we refer to as the model-space contribution (MSC) (58). We shall first consider this part.

We still assume that we operate to the far right on a function of the energy $\mathcal{E}$, and assume that the intermediate model-space state has the energy $\mathcal{E}'$. Specifying the energy parameter of the evolution operators, we can express the second-order evolution operator (169) as

$$U^{(2)}(t) = \mathrm{e}^{-\mathrm{i}t(\mathcal{E}-H_0)}\,U^{(1)}(0,\mathcal{E})\,U^{(1)}(0,\mathcal{E})P \tag{172}$$

and the counterterm, where the first factor is evolving from the intermediate state, as

$$C^{(2)}(t) = -\mathrm{e}^{-\mathrm{i}t(\mathcal{E}'-H_0)}\,U^{(1)}(0,\mathcal{E}')P \cdot PU^{(1)}(0,\mathcal{E})P \tag{173}$$

(Note that only the first factor of $C^{(2)}$ is time dependent, and that the time derivative eliminates the denominator of the leftmost resolvent for U as well as C.) This yields

$$\widetilde{U}^{(2)}(0)P = U^{(1)}(0,\mathcal{E})\,U^{(1)}(0,\mathcal{E})P - U^{(1)}(0,\mathcal{E}')P \cdot PU^{(1)}(0,\mathcal{E})P \tag{174}$$

and the evolution operator (76) with no intermediate model-space state

$$\bar{U}^{(2)}(0)P = U^{(1)}(0,\mathcal{E})\,Q\,U^{(1)}(0,\mathcal{E})P \tag{175}$$

The *model-space contribution* (MSC) (58) then becomes

$$M = U^{(1)}(0,\mathcal{E})\,P\,U^{(1)}(0,\mathcal{E})P + C^{(2)}(0)P = \Big(U^{(1)}(0,\mathcal{E})P - U^{(1)}(0,\mathcal{E}')P\Big)\cdot PU^{(1)}(0,\mathcal{E})P \tag{176}$$

The last factor is

$$PU^{(1)}(0,\mathcal{E})P = \frac{P}{\mathcal{E}-\mathcal{E}'}\,V(\mathcal{E})P = -\frac{1}{\delta\mathcal{E}} * PV(\mathcal{E})P = -\frac{1}{\delta\mathcal{E}} * P\dot{U}^{(1)}(\mathcal{E})P$$

with $\delta\mathcal{E} = \mathcal{E}' - \mathcal{E}$, and with $\delta U^{(1)} = U^{(1)}(0,\mathcal{E}') - U^{(1)}(0,\mathcal{E})$ we have

$$M = \Big(U^{(1)}(0,\mathcal{E})P - U^{(1)}(0,\mathcal{E}')P\Big)\cdot PU^{(1)}(0,\mathcal{E})P = \frac{\delta U^{(1)}}{\delta\mathcal{E}} * P\dot{U}^{(1)}P \tag{177}$$

(The asterisk is used only for clarity. It notifies the position of a "fold" in the graphical representation [47], but has no other special significance. It will mainly serve as a reminder of the position of a cancelled singularity, which—as we shall see—requires certain precautions.) With the definition (79) $P\dot{U}^{(1)}P = P\dot{\tilde{U}}^{(1)}P = H^{(1)}_{\text{eff}}$, which yields

$$M = \frac{\delta U^{(1)}}{\delta\mathcal{E}} * H^{(1)}_{\text{eff}} \tag{178}$$

The complete second-order reduced evolution operator (58) then becomes

$$\widetilde{U}^{(2)}(0)P = \bar{U}^{(2)}(0)P + \frac{\delta U^{(1)}}{\delta\mathcal{E}} * H^{(1)}_{\text{eff}} \tag{179}$$

The result above is exact also for the quasi-degenerate case. The difference ratio can be expanded as discussed in Appendix E

$$\frac{\delta U^{(1)}}{\delta\mathcal{E}} = \frac{\partial U^{(1)}}{\partial\mathcal{E}} + \frac{1}{2}\frac{\partial^2 U^{(1)}}{\partial\mathcal{E}^2}\,\delta\mathcal{E} + \frac{1}{3!}\frac{\partial^3 U^{(1)}}{\partial\mathcal{E}^3}\,\delta\mathcal{E}^2 + \cdots \tag{180}$$

which in the limit of complete degeneracy yields

$$\widetilde{U}^{(2)}(0)P = \bar{U}^{(2)}(0)P + \frac{\partial U^{(1)}}{\partial\mathcal{E}} * H^{(1)}_{\text{eff}} \tag{181}$$

The second-order contribution to the wave operator (66) then becomes

$$\boxed{\Omega^{(2)}P = Q\widetilde{U}^{(2)}(0)P = \bar{\Omega}^{(2)}P + \frac{\delta\Omega^{(1)}}{\delta\mathcal{E}} * H^{(1)}_{\text{eff}} \Rightarrow \bar{\Omega}^{(2)}P + \frac{\partial\Omega^{(1)}}{\partial\mathcal{E}} * H^{(1)}_{\text{eff}}} \tag{182}$$

where $\bar{\Omega}$ is the wave operator (91) without intermediate model space states.

The second-order contribution to the effective interaction is obtained by means of the relation (68). Since the expression (182) is valid only for $t = 0$, it can not be used to evaluate the time derivative. Instead, we have to use the original definition (170), and using the expressions (172) and (173), we find

$$H^{(2)}_{\text{eff}} = PV(\mathcal{E})\,\Gamma(\mathcal{E})\,V(\mathcal{E})P - PV(\mathcal{E}')\,\Gamma_P(\mathcal{E})\,V(\mathcal{E})P = \bar{H}^{(2)}_{\text{eff}} + \frac{\delta H^{(1)}_{\text{eff}}}{\delta\mathcal{E}} * \bar{H}^{(1)}_{\text{eff}} \tag{183}$$

where $\Gamma_P = P\Gamma$ and $\bar{H}^{(2)}_{\rm eff} = PV\Gamma_Q VP$ is the $H - bar$ operator (80) with no intermediate model-space states. The last term is by definition the model-space contribution, which appears in this order only for energy-dependent interactions. In the case of complete degeneracy the difference ratio tends to the derivative, as before,

$$\boxed{H^{(2)}_{\rm eff} = \bar{H}^{(2)}_{\rm eff} + \frac{\delta H^{(1)}_{\rm eff}}{\delta\mathcal{E}} * \bar{H}^{(1)}_{\rm eff} \Rightarrow \bar{H}^{(2)}_{\rm eff} + \frac{\partial H^{(1)}_{\rm eff}}{\partial\mathcal{E}} * \bar{H}^{(1)}_{\rm eff}} \tag{184}$$

D. Separable three-photon exchange

The treatment of the exchange of three separable covariant photons is quite analogous to the previous case. From the expansion (88) we have

$$\begin{aligned}\widetilde{U}^{(3)}P &= \bar{U}^{(3)}P + \big(\bar{U}^{(2)}PU^{(1)}P - \bar{U}^{(2)}P\cdot PU^{(1)}P\big) + \big(U^{(1)}P\bar{U}^{(2)}P - U^{(1)}P\cdot P\bar{U}^{(2)}P\big)\\ &+ \big(U^{(1)}PU^{(1)}P - U^{(1)}P\cdot PU^{(1)}P\big)\big(PU^{(1)}P - \cdot PU^{(1)}P\big)\end{aligned} \tag{185}$$

(Note that $U^{(1)} = \bar{U}^{(1)}$.) By generalizing the result of the preceding Appendix we obtain the relation

$$\boxed{AP\,BP - AP\cdot PBP = \frac{\delta A}{\delta\mathcal{E}} * P\dot{B}P} \tag{186}$$

where A is an arbitrary operator and B can be U, $\bar{U}$ or $\widetilde{U}$. Using this relation, the second and third terms above become

$$\big(\bar{U}^{(2)}PU^{(1)}P - \bar{U}^{(2)}P\cdot PU^{(1)}P\big) = \frac{\delta\bar{U}^{(2)}}{\delta\mathcal{E}} * P\dot{U}^{(1)}P = \frac{\delta\bar{U}^{(2)}}{\delta\mathcal{E}} * H^{(1)}_{\rm eff} \tag{187}$$

$$\big(U^{(1)}P\bar{U}^{(2)}P - U^{(1)}P\cdot P\bar{U}^{(2)}P\big) = \frac{\delta U^{(1)}}{\delta\mathcal{E}} * P\dot{\bar{U}}^{(2)}P = \frac{\delta U^{(1)}}{\delta\mathcal{E}} * \bar{H}^{(2)}_{\rm eff} \tag{188}$$

In the last term in Eq. (185) we have to apply the rule (186) twice, yielding

$$\begin{aligned}&\big(U^{(1)}PU^{(1)}P - U^{(1)}P\cdot PU^{(1)}P\big)\big(PU^{(1)}P - \cdot PU^{(1)}P\big)\\ =\;& \frac{\delta U^{(1)}}{\delta\mathcal{E}} * P\dot{U}^{(1)}P\,\big(PU^{(1)}P - \cdot PU^{(1)}P\big) = \frac{\delta}{\delta\mathcal{E}}\Big(\frac{\delta U^{(1)}}{\delta\mathcal{E}} * P\dot{U}^{(1)}P\Big) * P\dot{U}^{(1)}P\\ =\;& \frac{\delta}{\delta\mathcal{E}}\Big(\frac{\delta U^{(1)}}{\delta\mathcal{E}} * H^{(1)}_{\rm eff}\Big) * H^{(1)}_{\rm eff}\end{aligned} \tag{189}$$

From the previous Appendix (Eq. 179) we have

$$\frac{\delta\widetilde{U}^{(2)}}{\delta\mathcal{E}} = \frac{\delta\bar{U}^{(2)}}{\delta\mathcal{E}} + \frac{\delta}{\delta\mathcal{E}}\Big(\frac{\delta U^{(1)}}{\delta\mathcal{E}} * H^{(1)}_{\rm eff}\Big) \tag{190}$$

and the complete result then becomes

$$\widetilde{U}^{(3)}P = \bar{U}^{(3)}P + \frac{\delta\widetilde{U}^{(2)}}{\delta\mathcal{E}} * H^{(1)}_{\rm eff} + \frac{\delta U^{(1)}}{\delta\mathcal{E}} * \bar{H}^{(2)}_{\rm eff} \tag{191}$$

This is an exact expression in this order, also for a quasi-degenerate model space. In the case of complete degeneracy this becomes

$$\widetilde{U}^{(3)}P = \bar{U}^{(3)}P + \frac{\partial\widetilde{U}^{(2)}}{\partial\mathcal{E}} * H^{(1)}_{\rm eff} + \frac{\partial U^{(1)}}{\partial\mathcal{E}} * \bar{H}^{(2)}_{\rm eff} \tag{192}$$

In terms of the Ω operators the results above then become

$$\boxed{\Omega^{(3)}P = \bar{\Omega}^{(3)}P + \frac{\delta\Omega^{(2)}}{\delta\mathcal{E}} * H^{(1)}_{\rm eff} + \frac{\delta\Omega^{(1)}}{\delta\mathcal{E}} * \bar{H}^{(2)}_{\rm eff}} \tag{193}$$

In order to obtain the third-order effective interaction, we consider the time derivative of the relation (185) (only the first factor is time dependent). This yields

$$H^{(3)}_{\rm eff} = \bar{H}^{(3)}_{\rm eff} + \frac{\delta\bar{H}^{(2)}_{\rm eff}}{\delta\mathcal{E}} * H^{(1)}_{\rm eff} + \frac{\delta H^{(1)}_{\rm eff}}{\delta\mathcal{E}} * \bar{H}^{(2)}_{\rm eff} + \frac{\delta}{\delta\mathcal{E}}\Big(\frac{\delta H^{(1)}_{\rm eff}}{\delta\mathcal{E}} * H^{(1)}_{\rm eff}\Big) * H^{(1)}_{\rm eff} \tag{194}$$

which using the relation (184) can be expressed

$$\boxed{H^{(3)}_{\rm eff} = \bar{H}^{(3)}_{\rm eff} + \frac{\delta H^{(1)}_{\rm eff}}{\delta\mathcal{E}} * \bar{H}^{(2)}_{\rm eff} + \frac{\delta H^{(2)}_{\rm eff}}{\delta\mathcal{E}} * \bar{H}^{(1)}_{\rm eff}} \tag{195}$$

E. Expansions

We have seen above that when there are multiple singularities, it is important to take the difference ratios *before* the singularities are removed. We shall illustrate this here by a simple mathematical example.

We consider a function $f(x)$ of the variable x. We define the first-order difference ratio

$$\frac{\delta f}{\delta x} = \frac{\delta_{x_0,x} f}{\delta x} = \frac{f(x) - f(x_0)}{x - x_0} \tag{196}$$

which can be expanded in a Taylor series

$$\frac{\delta f}{\delta x} = \frac{\delta_{x_0,x} f}{\delta x} = f'(x_0) + \frac{1}{2}f"(x_0)(x-x_0) + \frac{1}{3!}f'''(x_0)(x-x_0)^2 + \frac{1}{4!}f^{IV}(x_0)(x-x_0)^3 + \cdots \tag{197}$$

where

$$f'(x_0) = \frac{\mathrm{d}f}{\mathrm{d}x}\Big|_{x=x_0} \tag{198}$$

etc.

Similarly, we define the second-order difference ratio

$$\begin{aligned}\frac{\delta^2 f}{\delta x^2} &= \frac{\delta_{x'x}}{\delta x}\frac{\delta_{x_0,x} f}{\delta x} = \frac{\frac{\delta_{x_0,x} f}{\delta x} - \frac{\delta_{x_0,x'} f}{\delta x}}{x - x'} = \frac{1}{2}f"(x_0) + \frac{1}{3!}f'''(x_0)(x + x' - 2x_0) \\ &+ \frac{1}{4!}f^{IV}(x_0)\big[(x' - x_0)^2 + (x' - x_0)(x - x_0) + (x - x_0)^2\big] + \cdots\end{aligned} \tag{199}$$

the third-order difference ratio

$$\frac{\delta^3 f}{\delta x^3} = \frac{\delta_{x"x}}{\delta x}\frac{\delta_{x'x}}{\delta x}\frac{\delta_{x_0,x} f}{\delta x} = \frac{1}{3!}f'''(x_0) + \frac{1}{4!}f^{IV}(x_0)(x + x' + x" - 3x_0) + \cdots \tag{200}$$

the fourth-order difference ratio

$$\frac{\delta^4 f}{\delta x^4} = \frac{1}{4!}f^{IV}(x_0) + \cdots \tag{201}$$

and so on.

Generalizing these results, we have in the limit, when the differences tend to zero

$$\boxed{\frac{\delta^n f}{\delta x^n} \Rightarrow \frac{1}{n!}\frac{\mathrm{d}^n f}{\mathrm{d}x^n}} \tag{202}$$

This relation is frequently used in the present paper.

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