Many-body-QED perturbation theory:
Connection to the Bethe-Salpeter equation

Ingvar Lindgren

Abstract: The connection between many-body theory (MBPT)—in perturbative and non-perturbative form—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 many-body perturbation theory. 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. It has the same relation to the BS equation as has the standard Bloch equation to the ordinary Schrödinger equation and can be used to generate a perturbation expansion compatible with the BS equation also for a quasi-degenerate model space.

PACS Nos.: 31.10+z, 31.15Md, 31.30Jv

Résumé: French version of abstract (supplied by CJP)
[Traduit par la rédaction]

Submitted 25 Jan. 2005, Corrected 8 Feb. 2005

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 4-dimensional wave function—with individual times for the two particles. This function is manifestly relativistically covariant but not in accordance with the 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 losing 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 to heliumlike ions, and we shall be particular concerned with the latter here. 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 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 $\alpha^5$ Ry (atomic units, or $m\alpha^2$ 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 order 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 non-perturbative but closely connected to MBPT, 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 at each order, which implies that the energy scales
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.

linearly with the size of the system—a property of vital importance for molecular problems [56, 57]. Both 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 techniques 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-times 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 non-perturbative coupled-cluster approach (CCA) of electron correlation or the so-called Dirac-Coulomb approximation, corresponding to the "ladder approximation" of the Bethe-Salpeter equation. This is combined with a perturbative 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—only in terms of BWPT, as has previously been the case [40, 44]. The Bloch equation in commutator form, compatible with the BS equation, which is 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—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 emphasize here is applications to atoms and other weak-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 then 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 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

\[ H \Psi = E \Psi \]  

(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). The Schrödinger equation can then be expressed

$$\begin{align*}
(E - H_0)\Psi &= V_1\Psi \\
\text{with the solution} \quad \Psi &= \Gamma(E)V_1, \\
\text{where} \quad \Gamma(E) &= \frac{1}{E - H_0} = \frac{|rs\rangle\langle rs|}{E - \varepsilon_r - \varepsilon_s}.
\end{align*}$$

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

$$h|i\rangle = \varepsilon_i|i\rangle \quad (5)$$

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 $\Lambda++$ 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 $V_1(E)$, i.e., Coulomb and transverse photon, the latter representing (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

$$\mathcal{V}(E) = V_1(E) + V_2(E) + \ldots \quad (6)$$

leads to

$$\Psi = \Gamma(E)\mathcal{V}(E)\Psi \quad (7)$$

or

$$\begin{align*}
(E - H_0)\Psi &= \mathcal{V}(E)\Psi \\
\text{This is equivalent to the Schrödinger-like form of the Bethe-Salpeter equation derived by Sucher [38, Eq. 1.47] and also used by Douglas and Kroll [40, 3.26] and by Zhang [43, Eq. 15].}
\end{align*}$$

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

$$\Psi = \Psi_0 + \left(\Gamma_Q(E)\mathcal{V}(E) + \Gamma_Q(E)\mathcal{V}(E)\Gamma_Q(E)\mathcal{V}(E) + \cdots\right)\Psi_0 \quad (9)$$

where $\Psi_0$ is the unperturbed wave function and

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

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 $\Psi_0$ and of the same symmetry. A rigorous derivation of the equation will be given in the following sections.

---

1 In this article relativistic units are used, i.e., $m = c = \hbar = \varepsilon_0 = 1$, $e^2 = 4\pi\alpha$, where $\alpha$ is the fine-structure constant.
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

\[ H \Psi^\alpha(x) = E^\alpha \Psi^\alpha(x); \quad (\alpha = 1, 2, \ldots, d) \]  

(\(x\) stands here for all space coordinates). The time-independent Hamiltonian is partitioned into a zeroth-order Hamiltonian and a perturbation

\[ H = H_0 + H' \]  

For each target state \(\Psi^\alpha(x)\) there exists a model state or zeroth-order wave function (ZOWF) \(\Psi^\alpha_0(x)\) that is confined to a subspace, the model space \((P)\), spanned by eigenfunctions 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 \(\Omega\) can be defined so that it transfers all model states to the corresponding target states

\[ \Psi^\alpha(x) = \Omega \Psi^\alpha_0(x); \quad (\alpha = 1, 2, \ldots, d) \]  

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

\[ \langle \Psi^\alpha_0(x) | \Psi^\alpha(x) \rangle = 1 \]  

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

\[ \Psi^\alpha_0(x) = P \Psi^\alpha(x) \]  

which implies

\[ P \Omega P = P \]  

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

\[ H_\text{eff} \Psi^\alpha_0(x) = E^\alpha \Psi^\alpha_0(x), \]  

within the model space. Here, \(H_\text{eff}\) is the effective Hamiltonian, in IN given by

\[ H_\text{eff} = P H \Omega P \]  

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

\[ [\Omega, H_0] P = (H' \Omega - \Omega H'_\text{eff}) P \]  

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

\[ H'_\text{eff} = H_\text{eff} - P H_0 P = P H' \Omega P \]  

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

\[ (E_0 - H_0) \Omega P = (H' \Omega - \Omega H'_\text{eff}) P \]  

The Bloch equation contains generally 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 and non-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) as well as the non-perturbative coupled-cluster approach (CCA). The
commutator form of the Bloch equation (19a) makes it possible to work with a non-degenerate or “ex-
tended” 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

\[ i \frac{\partial}{\partial t} \chi(t, x) = H(t) \chi(t, x) \]  

(20)

As before, \( x \) stands for all space coordinates, while \( t \) is a single time variable. Even if the Hamiltonian
may be formally time-dependent, we are interested in states that are stationary, which implies that the
wave function has the form

\[ \chi(t, x) = \Psi(x) e^{-iEt} \]  

(21)

where \( E \) is the energy of the system and \( \Psi(x) \) is the time-independent wave function. The latter is then
a solution the time-independent Schrödinger equation (2)

\[ H \Psi(x) = E \Psi(x) \]  

(22)

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

\[ \chi_I(t, x) = e^{iH_0 t} \chi(t, x) \]  

(23)

and the time-dependent Schrödinger equation becomes

\[ i \frac{\partial}{\partial t} \chi_I(t, x) = H'_I(t) \chi_I(t, x) \]  

(24)

The time-evolution operator, defined by

\[ \chi_I(t, x) = U_I(t, t_0) \chi_I(t_0, x) \]  

(25)

then satisfies the equation

\[ i \frac{\partial}{\partial t} U_I(t, t_0) = H'_I(t) U_I(t, t_0) \]  

(26)

with the solution [31, Eq. 6.23]

\[ U_I(t, t_0) = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^{t} dt' \int_{t_0}^{t} dt'' \cdot \cdot \cdot \int_{t_0}^{t} dt_N T_D [H'_I(t_n) \cdot \cdot \cdot H'_I(t_1)] \]  

(27)

Here, \( x = (t, x) \), \( T_D \) is the Dyson time-ordering operator, and \( H'_I(x) \) is the perturbation density defined by

\[ H'_I(t) = \int d^3x H'_I(t, x) \]  

(28)

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

\[ H'_I(t) \to H'_I e^{-\gamma t} ; \quad U_I(t, t_0) \to U_I(t, t_0) \]  

(29)
where \( \gamma \) is a small, positive number. This implies that as \( t \to -\infty \) 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]

\[
H_1(x) = -e \bar{\psi}_1(x) \alpha^\mu A_\mu(x) \psi_1(x)
\]

(30)

where \( e \) is the absolute value of the electronic charge, \( \bar{\psi}_1(x), \psi_1(x) \) are the electron-field operators in the interaction picture, \( A_\mu \) the photon-field operator and \( \alpha^\mu \) are related to the standard Dirac matrices by \( \alpha^\mu = (1, \alpha) \).

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 [31, pp. 64 and 116]

\[
G(x_1', x_2'; x_{10}, x_{20}) = -\frac{\langle 0_H| T_D \hat{\psi}_1(x_1') \hat{\psi}_1(x_2') \hat{\psi}_1(x_{20}) \hat{\psi}_1(x_{10}) |0_H \rangle}{\langle 0_H| 0_H \rangle}
\]

(31)

Here, \( |0_H \rangle \) represents the vacuum state and \( \hat{\psi}_1(x), \hat{\psi}_1(x) \) the electron-field operators, all in the Heisenberg representation. The latter are related to those in the interaction picture by

\[
\hat{\psi}_1(t, \varpi) = U(0, t) \hat{\psi}_1(t, \varpi) U(t, 0)
\]

(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]

\[
G(x_1', x_2'; x_{10}, x_{20}) = -\frac{\langle 0_H| T_D \hat{\psi}_1(x_1') \hat{\psi}_1(x_2') \hat{U}_1(\infty, -\infty) \hat{\psi}_1(x_{20}) \hat{\psi}_1(x_{10}) |0_H \rangle}{\langle 0_H| \hat{U}_1(\infty, -\infty) |0_H \rangle}
\]

(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]

\[
G(x_1', x_2'; x_{10}, x_{20}) = -\langle 0_H| T_D \hat{\psi}_1(x_1') \hat{\psi}_1(x_2') \hat{U}_1(\infty, -\infty) \hat{\psi}_1(x_{20}) \hat{\psi}_1(x_{10}) |0_H \rangle_{\text{conn}}
\]

(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

\[
G(x_1', x_2'; x_{10}, x_{20}) = G_0(x_1', x_2'; x_{10}, x_{20}) + \int \int \int \int d^4x_1 d^4x_2 d^4x_3 d^4x_4 G_0(x_1', x_2'; x_1, x_2) K(x_1, x_2; x_3, x_4) G_0(x_3, x_4; x_{10}, x_{20})
\]

(35)

where \( K \) represents the interaction kernel of all connected diagrams and \( G_0 \) is the zeroth-order Green’s function

\[
G_0(x_1', x_2'; x_{10}, x_{20}) = -\langle 0_H| T_D \hat{\psi}_1(x_1') \hat{\psi}_1(x_2') \hat{\psi}_1(x_{20}) \hat{\psi}_1(x_{10}) |0_H \rangle
= S_F(x_1', x_{10}) S_F(x_2', x_{20})
\]

(36)
with $S_F$ being the Feynman electron propagator or zeroth-order single-electron Green’s function, defined by

$$iS_F(x', x_0) = \langle 0_t | T_D [\hat{\psi}_I(x') \hat{\psi}_I^\dagger(x_0)] | 0_t \rangle$$

(37)

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

$$G = G_0 + G_0 \kappa G_0$$

(38)

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

$$\kappa = \kappa_2 G_0 \kappa_1$$

(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. The complete kernel can then be expressed

$$\kappa = \kappa + \kappa G_0 \kappa + \kappa G_0 \kappa G_0 \kappa + \cdots$$

(40)

where $\kappa$ represents all non-separable kernels. This leads to the Dyson equation for the Green’s function

$$G = G_0 + G_0 \kappa G$$

(41)

illustrated in Fig. 3.

**Fig. 2.** Graphical representation of the two-particle Green’s function (38). $\kappa$ represents all interactions between the electrons.

**Fig. 3.** Graphical representation of the Dyson equation (41) for the two-particle Green’s function. $\kappa$ represents the non-separable 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

---

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.
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

$$\Psi(x_1', x_2') = \int \int \int \int d^4x_1 d^4x_2 d^4x_3 d^4x_4 G_0(x_1', x_2'; x_1, x_2) \kappa(x_1, x_2; x_3, x_4) \Psi(x_3, x_4)$$

or in short-hand notations

$$\Psi = G_0 \kappa \Psi$$

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” $\kappa$ is by BS denoted by $\bar{G}$ and referred to as “irreducible graphs” and by GML denote 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 wave function (21) can in the case of a single target function be expressed in intermediate normalization (IN) (14) as

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

where $U_{\gamma}$ is the evolution operator (29) and $\Psi_0(x)$ is the time-independent zeroth-order wave function (15). (From now on we work in the interaction picture and leave out the subscript ”I”.) $\Psi(x)$ is an eigenfunction of the Hamiltonian $H_0 + H'$

$$(H_0 + H') \Psi(x) = E \Psi(x)$$

where $H'$ is in our case the electron-field interaction (30). Since this perturbation represents an uncontracted photon, the wave function $\Psi(x)$ 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]

$$\Psi^\alpha(x) = \lim_{\gamma \to 0} \frac{N^\alpha U_{\gamma}(0, -\infty)\Phi^\alpha(x)}{\langle \Phi^\alpha|U_{\gamma}(0, -\infty)|\Phi^\alpha \rangle}; \quad (\alpha = 1, 2, \ldots d)$$
where the function $\Phi^\alpha$ is defined

$$
\Phi^\alpha (\mathbf{x}) = \lim_{\gamma \to 0} \lim_{t \to -\infty} \chi^\alpha (t, \mathbf{x})
$$

(47)

This function is generally distinct from the zeroth-order wave function $\chi^0$ in intermediate normalization. Since the function (47) generally does not satisfy IN, a normalization constant $N^\alpha$ is inserted.

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

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

$$
U_{\text{Noncov}}(t' , t_0) = 1 + \hat{\psi}_+ \left( x_1' \right) \hat{\psi}_+ \left( x_2' \right) K \hat{\psi}_+ \left( x_2 \right) \hat{\psi}_+ \left( x_1 \right)
$$

(48)

where again $K$ represents the kernel of all fully contracted (separable and non-separable) interactions and $\hat{\psi}_+$, $\hat{\psi}_+$ 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]

$$
U_{\text{Cov}}(t' , t_0) = 1 + \int \int \int d^3 x_1' d^3 x_2' d^3 x_{10} d^3 x_{20} \hat{\psi}_+ \left( x_1' \right) \hat{\psi}_+ \left( x_2' \right) G_0 K G_0 \hat{\psi}_+ \left( x_2 \right) \hat{\psi}_+ \left( x_1 \right)
$$

(49)

leaving out the integrations over the coordinates of $K$ (see Eq. 35). It then follows from the relation (38) that the covariant evolution operator is related to the two-times Green’s function (where all initial
and all final times are equal) by

$$U_{\text{Cov}}(t', t_0) = \int \int \int \int d^3 x'_1 \, d^3 x'_2 \, d^3 x_{10} \, d^3 x_{20} \, \hat{\psi}^\dagger(x'_1) \hat{\psi}^\dagger(x'_2) \, G(x'_1, x'_2; x_{10}, x_{20}) \, \hat{\psi}(x_{20}) \hat{\psi}(x_{10})$$

(50)

as illustrated in Fig. 5 (right).

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

$$\int d^3 x_i S_F(x, x_0) \hat{\psi}(x_0) = \Theta(t - t_0) \hat{\psi}_+(x) - \Theta(t_0 - t) \hat{\psi}_-(x)$$

$$\int d^3 x \hat{\psi}^\dagger(x) S_F(x, x_0) = \Theta(t - t_0) \hat{\psi}^\dagger_+(x_0) - \Theta(t_0 - t) \hat{\psi}^\dagger_-(x_0)$$

(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 ”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 .2, 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 it 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 \( \tilde{U}(t, -\infty) \) [66, 64, Eq. 116], defined by

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

(52)

Here, the last term is a product of two operators that evolve independently from an initial state 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”

$$U(t, t_0) = U(t, t'') \, U(t'', t_0)$$

(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

\[ U(t)P = P + \tilde{U}(t)P \cdot PU(0)P \]  

(54)

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

\[ \tilde{U}(t)P = U'(t)P - \tilde{U}(t)P \cdot PU'(0)P \]  

(55)

Here, the last term is the counterterm

\[ C(t)P = -\tilde{U}(t)P \cdot PU'(0)P \]  

(56)

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

\[ C(t)P = -\tilde{U}(t)P \cdot P\tilde{U}(0)P - \tilde{U}(t)P \cdot P\tilde{U}(0)P \cdot P\tilde{U}(0)P - \cdots \]  

(57)

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

\[ MP = \tilde{U}(0)P - \bar{U}(0)P \]  

(58)

and further discussed in the Appendices. The new operator \( \tilde{U} \) (“\(U\)-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 .3, 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 (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

\[ U(t) = PU(t) + QU(t) \]  

(59)

where \( Q = 1 - P \) 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]

\[ U(0)P = [1 + Q\tilde{U}(0)]P \cdot PU(0)P \]  

(60)

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

\[ \Psi^\alpha(x) = [1 + Q\tilde{U}(0)] \Psi^\alpha_0 \]  

(61)

NRC Canada
where $\Psi_0^\alpha$ is the zeroth-order wave function (ZOWF) (15) in intermediate normalization
\[
\Psi_0^\alpha(x) = P\Psi^\alpha(x) = \frac{N^\alpha PU(0)\Phi^\alpha(x)}{\langle \Phi^\alpha|U(0)|\Phi^\alpha \rangle}
\]
(62)
The square bracket above is the wave operator
\[
\Omega = 1 + Q\tilde{U}(0)
\]
\[
\Psi^\alpha(x) = \Omega \Psi_0^\alpha(x)
\]
(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 $\Psi^\alpha$ 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
\[
P\Psi^\alpha(x) = P[1 + Q\tilde{U}(0)] \Psi_0^\alpha(x)
\]
(64)
or
\[
\Psi^\alpha(x) = [1 + Q\tilde{U}(0)]\Psi_0^\alpha(x)
\]
(65)
where $\Psi^\alpha(x) = P\Psi^\alpha(x)$ is the projected wave function on the restricted Hilbert space and $Q = PQ$ is the conventional projection operator for the complementary space (outside the model space). The wave operator in this space is
\[
\Omega = P\Omega = 1 + Q\tilde{U}(0)
\]
(66)
In IN (14) the wave operators satisfy in both spaces the relation (16)
\[
P\Omega P = P\Omega P = P.
\]
(67)
The effective interaction (19b) is in this formalism given by [64, Eq. 130]
\[
H_{\text{eff}}' = P\left[\frac{\partial}{\partial t}\tilde{U}(t)\right]_{t=0} P
\]
(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 wave function $\Psi^\alpha(x)$ 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 wave function $\Psi^\alpha = P\Psi^\alpha(x)$ 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 2 (Eq. 164), the contribution to the wave operator due the exchange of one single photon is
\[
\Omega^{(1)} P = Q\tilde{U}^{(1)}(0, \mathcal{E}) P = \Gamma_Q(\mathcal{E}) V(\mathcal{E}) P
\]
(69)
and the corresponding contribution to the effective Hamiltonian $H_{\text{eff}}^{(1)}(\mathcal{E}) = PV(\mathcal{E}) P$. Here, $\Gamma_Q(\mathcal{E})$ is the "reduced" resolvent (10) and $V(\mathcal{E})$ is the effective single-photon potential (162), assuming that we operate to the right on a fourier transform (157) with the energy parameter $\mathcal{E}$. 

NRC Canada
Similarly, it is demonstrated in Appendix .3 (Eq. 180) that the contribution to the evolution operator from two separable single-photon interactions is for a degenerate model space given by (leaving out the arguments)

\[
\Omega^{(2)} P = Q \tilde{U}^{(2)} P = \Gamma Q \Omega^{(1)} P + \frac{\partial \Omega^{(1)}}{\partial \mathcal{E}} * H_{\text{eff}}^{(1)}
\]

(70)

where the last term represents the model-space contribution (MSC) (58)

\[
QM^{(2)} P = \frac{\partial \Omega^{(1)}}{\partial \mathcal{E}} * H_{\text{eff}}^{(1)}
\]

(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 (182) due to two-photon exchange is

\[
H_{\text{eff}}^{(2)} = PV \Omega^{(1)} P + \frac{\partial H_{\text{eff}}^{(1)}}{\partial \mathcal{E}} * H_{\text{eff}}^{(1)} = \tilde{H}_{\text{eff}}^{(2)} + \frac{\partial H_{\text{eff}}^{(1)}}{\partial \mathcal{E}} * H_{\text{eff}}^{(1)}
\]

(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

\[
\frac{\partial H_{\text{eff}}^{(1)}}{\partial \mathcal{E}} * H_{\text{eff}}^{(1)} = P \frac{\partial V(\mathcal{E})}{\partial \mathcal{E}} \bigg|_{E_0} PV(E_0) P
\]

(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)

\[
\tilde{U}(t)P = \Gamma V P
\]

(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 also the time arguments, if there is no risk of ambiguity. We then express the counterterm (56) as

\[
CP = -\tilde{U} \cdot PU P
\]

(74)

and the evolution operator is given by

\[
UP = \Gamma V P + \Gamma VTV P + \Gamma VTVTV P + \cdots
\]

(75)

where \(\Gamma = \Gamma(\mathcal{E})\) is the resolvent (4). The "\(U\)-bar" operator (58), with all intermediate model-space states removed, is

\[
\tilde{U} P = \Gamma V P + \Gamma_{QV} V P + \Gamma_{QVTV} V P + \cdots
\]

(76)

We introduce a special symbol for the time derivative at time \(t = 0\)

\[
\dot{A} = \frac{\partial A}{\partial t} \bigg|_{t=0}
\]

(77)

Since the evolution operator (159) has the time dependence

\[
U(t, \mathcal{E}) = e^{-it(\mathcal{E} - H_0)} U(0, \mathcal{E})
\]

NRC Canada
it follows that the time derivation eliminates the denominator of the first (leftmost) resolvent, so that
\[ \dot{P}U_P = \dot{P}(V + VTQV + VTQVTQV + \cdots)P = PV_P + PVUP \]
\[ \dot{P}U_P = \dot{P}(V + VTQV + VTQVTQV + \cdots)P = PV_P + PVUP \quad (78) \]
The effective interaction \( H'_{\text{eff}} \) (68) is with this notation given by
\[ H'_{\text{eff}} = \dot{\tilde{P}}U_P \quad (79) \]
We also introduce the corresponding "H-bar" operator with no intermediate model-space states
\[ \tilde{H}'_{\text{eff}} = \dot{P}\tilde{U}P \quad (80) \]
We recall the definition (58) of the model-space contribution (MSC)
\[ \tilde{U}P = \tilde{U}P + MP \quad (81) \]
and can easily derive the identities
\[ U_P = \tilde{U}P + \tilde{U}PUP = \tilde{U}P + \tilde{U}PUP - M PUP \quad (82) \]
\[ \tilde{U}P = \tilde{U}P - \tilde{U}PUP + \tilde{U}PUP - \cdots \quad (83) \]
Then the reduced evolution operator (73) becomes
\[ \tilde{U}P = \tilde{U}P + CP = \tilde{U}P + \tilde{U}PUP - \tilde{U}PUP - M PUP \quad (84) \]
which using the definition (81) leads to the series
\[ \tilde{U}P = \tilde{U}P + (\tilde{U}PUP - \tilde{U}PUP)(1 - PUP + PUP - \cdots) \quad (85) \]
With the identity (83) this becomes
\[ \tilde{U}P = \tilde{U}P + (\tilde{U}PUP - \tilde{U}PUP) \quad (86) \]
which is an exact expression also for a quasi-degenerate model space. It can be expanded as
\[ \tilde{U}P = \tilde{U}P + (\tilde{U}PUP - \tilde{U}PUP)(PUP - \cdots) \quad (87) \]
As discussed in Appendix .3, the result (86) can be expressed
\[ \tilde{U}P = \tilde{U}P + \frac{\delta \tilde{U}}{\delta \epsilon} P\tilde{U}P = \tilde{U}P + \frac{\delta \tilde{U}}{\delta \epsilon} * \tilde{H}'_{\text{eff}} \quad (88) \]
where \( \delta \epsilon \) is the change in the model-space energy, represented by the "dot", \( \delta \tilde{U} \) is the corresponding change in \( \tilde{U} \), and \( \tilde{H}'_{\text{eff}} \) is the "H-bar" operator (80). In the case of complete degeneracy this becomes
\[ \tilde{U}P = \tilde{U}P + \frac{\partial \tilde{U}}{\partial \epsilon} \bigg|_{\epsilon = \epsilon_0} * \tilde{H}'_{\text{eff}} \quad (89) \]
Introducing the "Omega-bar" operator \( \tilde{\Omega} \) (with no intermediate model-space states) in analogy with the wave operator (66)
\[ \tilde{\Omega}P = P + Q\tilde{U}P = P + \Gamma QVP + \Gamma QVTQVP + \cdots \quad (90) \]
we can express the relations above as

$$\Omega P = \tilde{\Omega} P + \frac{\delta \Omega}{\delta \mathcal{E}} + \frac{\delta \Omega}{\delta \mathcal{E}} * \tilde{\Omega}' = \Omega P + \frac{\partial \Omega}{\partial \mathcal{E}} |_{\mathcal{E}=E_0} * \tilde{\Omega}'$$

(91)

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 (191).

By taking the time derivative of the relation (86), using the relations above, we obtain similarly

$$H'_\text{eff} = H'_\text{eff} + \frac{\delta H'_\text{eff}}{\delta \mathcal{E}} * H'_\text{eff} \Rightarrow \frac{\partial H'_\text{eff}}{\partial \mathcal{E}} |_{\mathcal{E}=E_0} * \tilde{\Omega}'$$

(92)

The second term represents here the model-space contribution to the effective interaction. This result agrees also with the third-order result (193).

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

$$\Omega P = \tilde{\Omega} P + \frac{\partial \tilde{\Omega}}{\partial \mathcal{E}} * H'_{\text{eff}} + \frac{\partial \tilde{\Omega}}{\partial \mathcal{E}} * \tilde{\Omega}' + \frac{\partial \tilde{\Omega}}{\partial \mathcal{E}} * (H'_{\text{eff}})^2 + \frac{3! \partial \tilde{\Omega}}{\partial \mathcal{E}} * (H'_{\text{eff}})^3 + \cdots = \Omega P + \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n \tilde{\Omega}}{\partial \mathcal{E}^n} * (H'_{\text{eff}})^n \text{ (93)}$$

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 (91) and (92), which we have rigorously derived. This equation contains eliminated singularities, indicated by the asterisks. As discussed in the Appendices, the derivative of such an expression has to be taken before the singularity is eliminated. Using the rules developed, particularly in Appendix 5, we find for instance

$$\frac{\partial}{\partial \mathcal{E}} \left( \frac{\delta \tilde{\Omega}}{\delta \mathcal{E}} * H'_{\text{eff}} \right) \Rightarrow \frac{1}{2} \frac{\partial^2 \tilde{\Omega}}{\partial \mathcal{E}^2} * H'_{\text{eff}} + \frac{\delta \tilde{\Omega}}{\delta \mathcal{E}} * \frac{\partial H'_{\text{eff}}}{\partial \mathcal{E}}$$

(94)

$$\frac{\partial}{\partial \mathcal{E}} \left( \frac{\delta^2 \tilde{\Omega}}{\delta \mathcal{E}^2} * \left( H'_{\text{eff}} \right)^2 \right) \Rightarrow \frac{1}{2} \frac{\partial^2 \tilde{\Omega}}{\partial \mathcal{E}^2} * \left( H'_{\text{eff}} \right)^2 + \frac{\delta \tilde{\Omega}}{\delta \mathcal{E}} * \frac{\partial H'_{\text{eff}}}{\partial \mathcal{E}} * H'_{\text{eff}} + \frac{1}{3!} \frac{\partial^3 \tilde{\Omega}}{\partial \mathcal{E}^3} * \left( H'_{\text{eff}} \right)^2 + \cdots$$

(95)

Note that in the second example the two $\tilde{\Omega}'$ 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 (93)

$$\frac{\partial \tilde{\Omega}}{\partial \mathcal{E}} = \frac{\partial \tilde{\Omega}}{\partial \mathcal{E}} + \frac{1}{2} \frac{\partial^2 \tilde{\Omega}}{\partial \mathcal{E}^2} * H'_{\text{eff}} + \frac{1}{3!} \frac{\partial^3 \tilde{\Omega}}{\partial \mathcal{E}^3} * \left( H'_{\text{eff}} \right)^2 + \cdots$$

$$+ \frac{\partial \tilde{\Omega}}{\partial \mathcal{E}} * \frac{\partial H'_{\text{eff}}}{\partial \mathcal{E}} + \frac{1}{2} \frac{\partial^2 \tilde{\Omega}}{\partial \mathcal{E}^2} * \frac{\partial H'_{\text{eff}}}{\partial \mathcal{E}} * H'_{\text{eff}} + \frac{1}{3!} \frac{\partial^3 \tilde{\Omega}}{\partial \mathcal{E}^3} * \frac{\partial H'_{\text{eff}}}{\partial \mathcal{E}} * \left( H'_{\text{eff}} \right)^2 + \cdots$$

(96)

or

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

(97)

We now insert this expression into the equation (91), which yields

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

(98)

or, using the relation (92),

$$\Omega P = \tilde{\Omega} P + \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n \tilde{\Omega}}{\partial \mathcal{E}^n} \left( H'_{\text{eff}} \right)^n$$

(99)

This is identical to the conjectured relation (91) and therefore completes the proof. The sum represents by definition the model-space contribution (MSC).
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

$$V(E) = V(E) + V_2(E) + V_3(E) + \cdots$$  \hspace{1cm} (100)

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

$$\bar{\Omega}F(E) = \bar{\Omega}(E)F(E)$$  \hspace{1cm} (101)

For a degenerate model space of energy $E_0$ this means that

$$\bar{\Omega}P = \bar{\Omega}(E_0)P = P + \Gamma Q(E_0)\mathcal{V}(E_0) + \cdots$$  \hspace{1cm} (102)

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),

$$H'_{\text{eff}}|\Psi_0^\alpha\rangle = \Delta E^\alpha |\Psi_0^\alpha\rangle$$  \hspace{1cm} (103)

where $\Delta E^\alpha = E^\alpha - E_0$. Operating with the operator equation (99) directly on the model function $\Psi_0^\alpha$ then leads to the Taylor expansion

$$\Omega\Psi_0^\alpha = \left[\bar{\Omega}(E_0) + \frac{\partial \bar{\Omega}}{\partial E} |_{E_0} \Delta E^\alpha + \frac{1}{2} \frac{\partial^2 \bar{\Omega}}{\partial^2 E} |_{E_0} (\Delta E^\alpha)^2 + \frac{1}{3!} \cdots \right] \Psi_0^\alpha = \bar{\Omega}(E^\alpha)\Psi_0^\alpha$$  \hspace{1cm} (104)

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 $E^\alpha$. But $\bar{\Omega}(E^\alpha)\Psi_0^\alpha$ with the energy parameter equal to the full energy for the state $\Psi^\alpha$ is also identical to the Brillouin-Wigner expansion (9),

$$\bar{\Omega}(E^\alpha)\Psi_0^\alpha = \left[1 + \frac{Q}{E^\alpha - H_0} \mathcal{V}(E^\alpha) + \frac{Q}{E^\alpha - H_0} \mathcal{V}(E^\alpha) \frac{Q}{E^\alpha - H_0} \mathcal{V}(E^\alpha) + \cdots \right] \Psi_0^\alpha$$  \hspace{1cm} (105)
which represents the full wave function, i.e.,
\[
\Omega(E^\alpha)\Psi_0^\alpha = \Omega_0^\alpha \tag{106}
\]
This implies that the relation (99) 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 arrow in the diagram of Fig. 1).

The BW expansion (105) can be expressed
\[
\Omega_0^\alpha = \Psi_0^\alpha + \Gamma_0^\alpha (E^\alpha) \mathcal{V}(E^\alpha) \Omega_0^\alpha \tag{107}
\]
or
\[
(E^\alpha - H_0^\alpha) Q \Psi_0^\alpha = Q \mathcal{V}(E^\alpha) \Psi_0^\alpha \tag{108}
\]

From the relation (92) it can be shown in analogy with the relation (99)
\[
H'_\text{eff} = \tilde{H}'_\text{eff} + \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n \tilde{H}'_\text{eff}}{\partial E^n} (H'_\text{eff})^n \tag{109}
\]
With the definitions (80) and (90) this leads to
\[
\tilde{H}'_\text{eff} = P \mathcal{V}(E_0^\alpha) \tilde{\Omega}(E_0^\alpha) P \tag{110}
\]
and in analogy with the relation (104) to
\[
H'_\text{eff} = P \mathcal{V}(E^\alpha) \tilde{\Omega}(E^\alpha) P = P \mathcal{V}(E^\alpha) \Omega P \tag{111}
\]
This leads together with Eq. (108) to the final equation
\[
(E^\alpha - H_0^\alpha) \Psi_0^\alpha = \mathcal{V}(E^\alpha) \Psi_0^\alpha \tag{112}
\]
This is the Bethe-Salpeter equation for energy-dependent interactions in the Schrödinger-like form (8).

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 (30), corresponds in the projected Hilbert space with no uncontracted photons to a Schrödinger-like equation with the perturbation (100). 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 (139) is merged with the kernel \( \kappa \) to form the potential \( \mathcal{V} \).

The Schrödinger-like equation (112) 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-times” 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 (103) simplifies the treatment, and the formulas derived in the previous section lead directly to the standard Bethe-Salpeter equation (112). 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 be derived by induction

$$\frac{\partial^n Q}{\partial E^n} = \Gamma_Q \frac{\partial^n (\nabla Q)}{\partial E^n} - n\Gamma_Q \frac{\partial^{(n-1)} Q}{\partial E^{(n-1)}}$$  \hspace{1cm} (113)

To prove this we form the next-order derivative

$$\frac{\partial^{(n+1)} Q}{\partial E^{(n+1)}} = -\Gamma^2 Q \frac{\partial^n (\nabla Q)}{\partial E^n} + \Gamma_Q \frac{\partial^{(n+1)} (\nabla Q)}{\partial E^{(n+1)}} + n\Gamma_Q \frac{\partial^{(n+1)} (\nabla Q)}{\partial E^{(n+1)}} - n\Gamma_Q \frac{\partial^n Q}{\partial E^n}$$

(Since no singularities are involved here, ordinary rules of derivation can be used.) Inserting the expression (113) in the first term, yields

$$\frac{\partial^{(n+1)} Q}{\partial E^{(n+1)}} = \Gamma_Q \frac{\partial^{(n+1)} (\nabla Q)}{\partial E^{(n+1)}} - (n+1)\Gamma_Q \frac{\partial^n Q}{\partial E^n}$$

In first order we have with $\Omega = 1 - \Gamma_Q \nabla Q$

$$\frac{\partial \Omega}{\partial E} = \Gamma_Q \frac{\partial (\nabla Q)}{\partial E} - \Gamma_Q \bar{\Omega}$$

which completes the proof of the relation (113).

The formula above leads together with the expansion (99) to

$$Q\bar{\Omega}P = Q\bar{\Omega}P + \Gamma_Q \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n (\nabla Q)}{\partial E^n} \left( H'_{\text{eff}} \right)^n - \Gamma_Q \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \frac{\partial^{(n-1)} Q}{\partial E^{(n-1)}} \left( H'_{\text{eff}} \right)^n \hspace{1cm} (114)$$

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

$$Q\bar{\Omega}P = \Gamma_Q \nabla Q \bar{\Omega}P + \Gamma_Q \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n (\nabla Q)}{\partial E^n} \left( H'_{\text{eff}} \right)^n - \Gamma_Q \Omega H'_{\text{eff}} \hspace{1cm} (115)$$

We can consider $\nabla Q \bar{\Omega}$ 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

$$\nabla (E_0) \bar{\Omega} (E_0) + \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n (\nabla Q)}{\partial E^n} \bigg| \left[ \Delta E^\alpha \right]^n = \nabla (E^\alpha) \bar{\Omega} (E^\alpha). \hspace{1cm} (116)$$

Thus, the expansion has the effect of transforming the energy parameter of the product $\nabla Q \bar{\Omega}$ from $E_0$ to the full energy $E^\alpha$, 

$$\nabla (E_0) \bar{\Omega} (E_0) \Psi_0^\alpha \rightarrow \nabla (E^\alpha) \bar{\Omega} (E^\alpha) \Psi_0^\alpha \hspace{1cm} (117)$$

in analogy with the expansion (105). Using the relation (106), the equation (115) above then becomes

$$Q\bar{\Omega} \Psi_0^\alpha = \Gamma_Q \left[ \nabla (E^\alpha) \bar{\Omega} - \frac{\Delta E^\alpha}{H'_{\text{eff}}} \right] \Psi_0^\alpha \hspace{1cm} (118)$$

NRC Canada
or
\[(E_0 - H_0)\Psi^\alpha_0 = Q \left[ \mathcal{V}(E^{\alpha})\Omega - \Omega H'_\text{eff} \right] \Psi^\alpha_0 \quad (119)\]
which is consistent with the Bethe-Salpeter equation (112).

If the model space is non-degenerate (quasi-degenerate), then the relation (103) is no longer valid, and the expansion (115) can not be expressed by means of a single energy parameter as in the Taylor expansion (116). Instead, the potential will depend on the full matrix of the effective Hamiltonian. We then replace the energy parameter in (102) 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 (101)—
\[A(H_0)B\Phi = A(E_0)B\Phi \quad (120)\]
when \(\Phi\) is an eigenfunction of \(H_0\) with the eigenvalue \(E_0\) and \(B\) is an arbitrary operator combination. Together with the linearity condition,
\[A(H_0)B(a\Phi + b\Phi') = aA(E_0)B\Phi + bA(E'_0)B\Phi' \quad (121)\]
where \(\Phi'\) is another eigenfunction of \(H_0\) with the eigenvalue \(E'_0\), this defines the notation fully.

The expansion (115) can now be regarded, in analogy with the energy modification (116), as modifying the parameter \(H_0\) to the full effective Hamiltonian \(H_{\text{eff}} = H_0 + H'_{\text{eff}}\)
\[\mathcal{V}(H_0) \bar{\Omega}(H_0) + \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n(\bar{\Omega})}{\partial E^n} (H'_{\text{eff}})^n = \mathcal{V}(H_{\text{eff}}) \bar{\Omega}(H_{\text{eff}}) \quad (122)\]
i.e.,
\[\mathcal{V}(H_0)\bar{\Omega}(H_0) P \rightarrow \mathcal{V}(H_{\text{eff}})\bar{\Omega}(H_{\text{eff}}) P \quad (123)\]
and Eq. (118) becomes
\[Q\Omega P = \Gamma_Q(H_0)\mathcal{V}(H_{\text{eff}})\bar{\Omega}(H_{\text{eff}}) P - \Gamma_Q(H_0)\Omega H'_{\text{eff}} \quad (124)\]
The notation here is defined by the relation
\[A(H_{\text{eff}})B\Psi^\alpha_0 = A(E^{\alpha})B\Psi^\alpha_0 \quad (125)\]
where \(\Psi^\alpha_0\) is a model function (eigenfunction of \(H_{\text{eff}}\) with the eigenvalue \(E^{\alpha}\), see Eq. 17), which together with the linearity condition defines the operator when acting on any model space.

Similarly, the expansion (99) yields
\[\Omega P = \bar{\Omega}(H_0) P + \sum_{n=1}^{\infty} \frac{1}{n!} \frac{\partial^n(\bar{\Omega})}{\partial E^n} (H'_{\text{eff}})^n = \bar{\Omega}(H_{\text{eff}}) P \quad (126)\]
and we can now express the equation (124) as
\[Q\Omega P = \Gamma_Q(H_0)\mathcal{V}(H_{\text{eff}}) \Omega P - \Gamma_Q(H_0)\Omega H'_{\text{eff}} \quad (127)\]
or
\[\Gamma_Q(H_0)]^{-1} Q\Omega P = Q \left[ \mathcal{V}(H_{\text{eff}}) \Omega - Q\Omega H'_{\text{eff}} \right] P \quad (128)\]
Operating on a model-state function \(\Phi(E^{\alpha}_0)\) of energy \(E^{\alpha}_0\), we have according to the definitions above
\[\Gamma_Q(H_0)]^{-1} \Phi(E^{\alpha}_0) = (E^{\alpha}_0 - H_0) \Omega \Phi(E^{\alpha}_0) \quad (129)\]

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

\[ \left[ \Gamma_Q(H_0) \right]^{-1} A \equiv [A, H_0] \]  

(129)

where \( A \) is an arbitrary operator. This leads to the commutator relation

\[ [\Omega, H_0] P = Q \mathcal{V}(H_{\text{eff}}) \Omega P - Q \Omega H'_{\text{eff}} \]  

(130)

The relation (111) can be generalized to

\[ H'_{\text{eff}} = P \mathcal{V}(H_{\text{eff}}) \Omega P \]  

(131)

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

\[ [\Omega, H_0] P = \mathcal{V}(H_{\text{eff}}) \Omega P - \Omega H'_{\text{eff}} \]  

(132)

The equation above—which we shall refer to as the Bethe-Salpeter-Bloch equation—is the main result of the present work. It has the same relation to the standard BS equation as has the standard Bloch equation (19a) to the ordinary Schrödinger equation. It can be used to generate the BS equation perturbatively, essentially as the ordinary Bloch equation is used in standard MBPT. The commutator form makes it possible to apply the equation to an extended model space, which essentially eliminates the quasi-degeneracy problem that might appear in applying the standard equation directly on a single state.

5.4. Expansion of the Bethe-Salpeter-Bloch equation

The original Bethe-Salpeter equation contains the exact energy and is therefore normally treated by means a Brillouin-Wigner perturbation expansion [40, 44], which requires a self-consistent treatment. The BS equation in the Bloch-equation form can be used to generate a perturbation expansion of Rayleigh-Schrödinger type that does not require any self-consistence procedure. We have at our laboratory developed a procedure of solving the Bethe-Salpeter-Bloch equation that is a combination of perturbative and non-perturbative techniques, which we shall here briefly indicate. A detailed description of the procedure together with numerical results will appear shortly [74].

Our procedure is based upon the iterative solution of pair equations [75, 76, 77, 78, 47]. This represents the "ladder" approximation of the BS equation, as indicated in Fig. 7 (a). The pair function

NRC Canada
is combined with the emission of a single (uncontracted) photon (Fig. 7 b). This represents a function in the extended Fock space, discussed in section 4.3. This function can be iterated further, before the photon is annihilated, which can yield instantaneous (Coulomb and Breit) interactions, crossing the photon. These iterations can be continued after the annihilation, as indicated in Fig. 7 (c). By annihilating the photon on the same electron line, leads to self-energy and vertex corrections (Fig. 7 d). At present time it is possible to treat only one covariant photon in this way, but the dominating part of the multi-photon exchange will be included by the crossings with the instantaneous interactions (c). This will correspond to all effects treated by Zhang [44] in his analysis of the helium fine structure up to order $m^7$, except for the non-separable part of two-photon exchange (Fig. 6). With our approach this part has at present to be included analytically.

6. Summary and conclusions

Standard many-body perturbation theory (MBPT) is conveniently based upon the Bloch equation, which is the generating equation for 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 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 and non-perturbative schemes, based upon Rayleigh-Schrödinger perturbation theory and schemes based upon the BS equation, which are normally treated by means of Brillouin-Wigner perturbation theory.

In addition, a Bloch equation in commutator form that is compatible with the BS equation is derived. This 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. This can be used to generate a perturbative expansion, corresponding to the BS equation for an extended model space. In principle, this will make it possible to treat the quasi-degeneracy problem also within the BS formalism. Such a scheme is presently being tested at our laboratory.

Acknowledgements

The author wish to express his gratitude to Sten Salomonson, Ann-Marie Pendrill, Björn Åsén and Daniel Hedendahl for the collaboration on which the work presented here is largely based. Stimulating discussions with Gordon Drake has been particular valuable for this work and gratefully acknowledged.
APPENDIX

1. Zeroth-order Green’s function

The zeroth-order Green’s function (36) in Fig. 8 is in coordinate representation

\[ G_0(x_1 x_2; x_{10} x_{20}) = S_F(x_1; x_{10}) S_F(x_2; x_{20}) \]  \hspace{1cm} (133)

where \( S_F \) is the electron propagator

\[ S(x, x_0) = \int \frac{d\omega}{2\pi} S(\omega) e^{-i\omega(t-t_0)} \]  \hspace{1cm} (134)

with the fourier transform

\[ \langle x|S(\omega)|x_0\rangle = \frac{\langle x|r \rangle \langle r|x_0\rangle}{\omega - \epsilon_r + i\eta_r} = \langle x|\hat{S}(\omega)|x_0\rangle \]  \hspace{1cm} (135)

and the corresponding operator form

\[ \hat{S}(\omega) = \frac{\Lambda_+}{\omega - h + i\eta} + \frac{\Lambda_-}{\omega - h - i\eta} \]  \hspace{1cm} (136)

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

\[ G_0(t, x_1, x_2; x_{10}, x_{20}) = \int \frac{d\epsilon}{2\pi} e^{-i\epsilon t} \frac{\langle x_1 x_2 | rs \rangle \langle rs | x_{10} x_{20} \rangle}{\epsilon - \epsilon_s - \epsilon_r} \] 
\[ \times \int \frac{d\omega}{2\pi} \left[ \frac{1}{\omega - \epsilon_r + i\eta_r} + \frac{1}{\epsilon - \omega - \epsilon_s + i\eta_s} \right] e^{i\omega t_{10}} e^{i(\epsilon - \omega) t_{20}} \]  \hspace{1cm} (137)

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

\[ G_0(\epsilon, x_1, x_2; x_{10}, x_{20}) = \frac{\langle x_1 x_2 | rs \rangle \langle rs | x_{10} x_{20} \rangle}{\epsilon - \epsilon_s - \epsilon_r} \] 
\[ \int \frac{d\omega}{2\pi} \left[ \frac{1}{\omega - \epsilon_r + i\eta_r} + \frac{1}{\epsilon - \omega - \epsilon_s + i\eta_s} \right] e^{i\omega t_{10}} e^{i(\epsilon - \omega) t_{20}} \]  \hspace{1cm} (138)

or in operator form

\[ G_0(\epsilon) = \Gamma(\epsilon) \int \frac{d\omega}{2\pi} g_0(\epsilon, \omega) e^{i\omega t_{10}} e^{i(\epsilon - \omega) t_{20}} \]  \hspace{1cm} (139)
Lindgren

where $\Gamma(E)$ is the resolvent (4)

$$\Gamma(E) = \frac{1}{E - H_0}$$  \hspace{1cm} (140)

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

$$g_0(\epsilon, \omega) = \Lambda + \left[ \frac{1}{\omega - h_1 + i\eta} - \frac{1}{\epsilon - h_1 + i\eta} \right]$$

$$+ \Lambda - \left[ \frac{1}{\omega - h_1 - i\eta} - \frac{1}{\epsilon - h_1 - i\eta} \right]$$  \hspace{1cm} (141)

The inverse transformation is

$$G_0(t, x_1, x_2; x_{10}, x_{20}) = \int \frac{d\epsilon}{2\pi} e^{-\imath \epsilon t} G_0(\epsilon, x_1, x_2; x_{10}, x_{20})$$  \hspace{1cm} (142)

and specifically,

$$G_0(t = 0, x_1, x_2; x_{10}, x_{20}) = \int \frac{d\epsilon}{2\pi} G_0(\epsilon, x_1, x_2; x_{10}, x_{20})$$  \hspace{1cm} (143)

### 2. Single-photon exchange

(See Ref. [64, Eq. 312].) We consider now the covariant evolution operator (49) for the exchange of a single-photon, represented by the diagram in Fig. 9 (left)

$$U^{(1)}(t', t_0) = -\frac{1}{2} \int \int d^3x'_1 d^3x'_2 \hat{\psi}^\dagger(x'_1) \hat{\psi}^\dagger(x'_2) \int \int d^4x_1 d^4x_2 iS_F(x'_1, x_1) iS_F(x'_2, x_2) iI(x_2, x_1)$$

$$\times \int \int d^3x_{10} d^3x_{20} iS_F(x_1, x_{10}) iS_F(x_2, x_{20}) \hat{\psi}(x_{10}) \hat{\psi}(x_{10})$$  \hspace{1cm} (144)

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

$$U^{(1)}(t', t_0) = -\frac{1}{2} \hat{\psi}^\dagger(x'_1) \hat{\psi}^\dagger(x'_2) G_0(x'_1, x'_2; x_1 x_2) iI(x_2, x_1)$$

$$\times G_0(x_1, x_2; x_{10} x_{20}) \hat{\psi}(x_{10}) \hat{\psi}(x_{10})$$  \hspace{1cm} (145)

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

$$I(x_2, x_1) = e\alpha^\mu D_{\mu\nu}(x_2 - x_1) e\alpha^\nu = \int \frac{dz}{2\pi} e^{-i(z - t_1)} I(z, x_2, x_1)$$  \hspace{1cm} (146)

where $D_{\mu\nu}(x_2 - x_1)$ is the Feynman photon propagator.

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

$$U^{(1)}(t', -\infty) = \frac{1}{2} \hat{\psi}^\dagger(x'_1) \hat{\psi}^\dagger(x'_2) G_0(x'_1, x'_2; x_1 x_2) iI(x_2, x_1) \hat{\psi}(x_2) \hat{\psi}(x_1)$$  \hspace{1cm} (147)

The electron-field operator is in the interaction picture [31]

$$\hat{\psi}(x) = \hat{\psi}(t, x) = c_j \phi_j(x) e^{-i\epsilon_j t}$$  \hspace{1cm} (148)
An arbitrary function of any electron-electron interaction. Thus, Fig. 9, yields

\[
\text{(150), yields}
\]

Operating on a (time-independent) fourier component with the electron-field operator

\[ \psi \] 

With the adiabatic damping the time-independent component corresponds to the field operator propagates the function \( \psi(x) \) operating on a time-independent two-electron function, which implies that the field operator propagates the function \( F(\omega_1, x_1) \) from the time \(-\infty\) to \( t \). Similarly, the product of two electron-field operators \( \psi(x_1)\hat{\psi}(x_2) \) operating on a time-independent two-electron function, propagates the individual electrons from the time \( t = -\infty \) to \( t = t_1 \) and \( t = t_2 \), respectively, without any electron-electron interaction. Thus,

\[
\psi(x_1)\hat{\psi}(x_2) F(\omega_1, \omega_2) = e^{-it_1 \omega_1} e^{-it_2 \omega_2} F(\omega_1, \omega_2)
\]  

We now use the form (142) of the Green’s function

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

to operate with the evolution operator (147) on the fourier component \( F(\omega_1, \omega_2) \) (see also Fig. 9, right), which yields

\[
U^{(1)}(t', -\infty) F(\omega_1, \omega_2) = \frac{1}{2} c_i^j \phi_j(\epsilon) c_i^k \phi_k(\omega) e^{it' \epsilon} \Gamma(\epsilon) F(\omega_1, \omega_2)
\]

\[
\times \int \frac{d\omega}{2\pi} g_0(\epsilon, \omega) \int \frac{dz}{2\pi} i F(z) e^{-it_1(\omega_1 - z - \omega)} e^{-it_2(\omega_2 + z - \epsilon + \omega)} F(\omega_1, \omega_2)
\]  

Fig. 9. Graphical representation of the covariant-evolution operator for single-photon exchange in the form (144) (left) and in the form (147) with \( t_0 \to -\infty \) (right).
and after time integrations
\[
U^{(1)}(t', -\infty) F(\omega_1, \omega_2) = |rs\rangle\langle rs| \int \frac{d\omega}{2\pi} e^{-it'(\epsilon - \epsilon_r - \epsilon_s)} \Gamma(\epsilon) \int \frac{d\omega}{2\pi} g_0(\epsilon, \omega) \int \frac{dz}{2\pi} iF(z) \\
\times F(\omega_1, \omega_2) 2\pi\delta(\omega_1 - z - \omega) 2\pi\delta(\omega_1 + \omega_2 - \epsilon)
\]
(156)

Here, \(|ij\rangle\) represents a straight (non-symmetrized) product of time-independent single-electron functions (which eliminates the factor of \(\frac{1}{2}\)).

If we operate on a particular energy component
\[
F(\epsilon) = \int \frac{d\omega_1}{2\pi} F(\omega_1, \epsilon - \omega_1)
\]
the result becomes in operator form
\[
U^{(1)}(t', -\infty) F(\epsilon) = e^{-it'(\epsilon - H_0)} \Gamma(\epsilon) \int \frac{d\omega}{2\pi} g_0(\epsilon, \omega) \int \frac{d\omega_1}{2\pi} iF(\omega_1 - \epsilon) F(\epsilon) \\
\times \int \frac{d\omega_1}{2\pi} iF(\omega_1 - \epsilon) F(\epsilon - \omega_1)
\]
(158)

We can also express this result as
\[
U^{(1)}(t, -\infty) F(\epsilon) = e^{-it(\epsilon - H_0)} \Gamma(\epsilon) V(\epsilon) F(\epsilon)
\]
(159)

where
\[
V(\epsilon) = \int \frac{d\omega}{2\pi} g_0(\epsilon, \omega) \int \frac{d\omega_1}{2\pi} iF(\omega_1 - \epsilon)
\]
(160)

Here, \(\Gamma(\epsilon)\) is the resolvent (140) and \(g_0(\epsilon, \omega)\) is the operator (141). The corresponding effective interaction is obtained from the relation (68) by taking the time derivative at \(t = 0\), which eliminates the resolvent,
\[
H_{\text{eff}}^{(1)}(\epsilon) = PV(\epsilon) P
\]
(161)

With the explicit form of the interaction (146) the matrix elements of the potential for the exchange of a single covariant photon becomes [64, App. A]
\[
\langle rs|V(\epsilon)|tu\rangle = \langle rs| \int f(k)dk \left[ \frac{1}{\epsilon - \epsilon_r - \epsilon_u - (k - i\gamma)_r} + \frac{1}{\epsilon - \epsilon_s - \epsilon_t - (k - i\gamma)_s} \right] |tu\rangle
\]
(162)

where the \(A_r = A \text{sgn}(\epsilon_r)\). The function \(f(k)\) is in the Feynman gauge given by [64, Eq. 77]
\[
f(k) = -\frac{e^2}{4\pi^2} (1 - \alpha_1 \cdot \alpha_2) \frac{\sin(kr_{12})}{r_{12}} \\
\quad = -\frac{e^2}{4\pi^2} (1 - \alpha_1 \cdot \alpha_2) \sum_{l=0}^{\infty} (2l + 1) j_l(kr_{1}) j_l(kr_{2}) C^{(k)}(1) \cdot C^{(k)}(2)
\]
(163)

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

Summarizing, the contribution to the wave operator (65) from single-photon exchange, when operating to the right on a function of the type (157), becomes
\[
\Omega^{(1)}(\epsilon) = Q\tilde{U}^{(1)}(0, -\infty) = \Gamma(\epsilon)V(\epsilon)
\]
(164)

NRC Canada
where
\[ \Gamma_Q(\mathcal{E}) = Q \Gamma(\mathcal{E}) = \frac{Q}{\mathcal{E} - H_0} \] (165)
and the corresponding contribution to the effective Hamiltonian
\[ H_{\text{eff}}^{(1)}(\mathcal{E}) = PV(\mathcal{E}) P \] (166)

3. 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. 10 (left). The evolution operator (25) can in this case be expressed
\[ U^{(2)}(t, -\infty)P = U^{(1)}(t, t'') U^{(1)}(t'', -\infty)P \] (167)
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 including counterterms (56)
\[ \tilde{U}(t)P = U(t)P + C(t)P \] (168)
We also recall the definition of the model-space contribution (MSC) (58)
\[ \tilde{U}(0)P = \tilde{U}(0)P + MP \] (169)
where \( \tilde{U} \) is the evolution operator (76) with no intermediate model-space state, in this case
\[ \tilde{U}^{(2)}P = \Gamma V T Q V P \] (170)
The counterterm (56) is in the present case given by the product of two single-photon contributions,

\[ C^{(2)}(t) = -U^{(1)}(t, -\infty) \cdot P U^{(1)}(0, -\infty)P = -U^{(1)}(t) \cdot P U^{(1)}(0) \] (171)

Fig. 10. 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.

as shown in Fig. 10 (right)
using the notation introduced in subsection 4.2. 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 \textit{finite remainder}, which we refer to as the model-space contribution (MSC) \eqref{eq:169}. We shall first consider this part.

We assume that we operate to the far right on a function of the type \eqref{eq:157} of energy $E$, and that the intermediate model-space state has the energy $E'$. Using the first-order result \eqref{eq:159}, we can express the second-order evolution operator \eqref{eq:167} as

\begin{equation}
U^{(2)}(t)P = e^{-i(E - H_0) t} U^{(1)}(0, E) U^{(1)}(0, E) P
\end{equation}

and the counterterm—with the first factor evolving from the intermediate state—as

\begin{equation}
C^{(2)}(t) = -e^{-i(E' - H_0) t} U^{(1)}(0, E') \cdot P U^{(1)}(0, E) P
\end{equation}

We note here that the time derivative for $U$ as well as $C$ eliminates the denominator of the leftmost resolvent.

The MSC now becomes

\begin{equation}
MP = \left(U^{(1)}(0, E) - U^{(1)}(0, E')\right) \cdot P U^{(1)}(0, E) P
\end{equation}

Using the result \eqref{eq:78}, the last factor is

\begin{equation}
PU^{(1)}(0, E)P = \frac{P}{E - E'} V(E) P = -\frac{1}{\delta E} \ast PV^{(1)}(E) P = -\frac{1}{\delta E} \ast P\dot{U}^{(1)}(E) P
\end{equation}

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

\begin{equation}
MP = \left(U^{(1)}(0, E) - U^{(1)}(0, E')\right) \cdot P U^{(1)}(0, E) P = \frac{\delta U^{(1)}}{\delta E} \ast P\dot{U}^{(1)} P
\end{equation}

(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 \eqref{eq:80} the MSC can be expressed

\begin{equation}
MP = \frac{\delta U^{(1)}}{\delta E} \ast H^{(1)}_{\text{eff}}
\end{equation}

(Note that $\bar{U}^{(1)} = U^{(1)}$ and $\bar{H}^{(1)}_{\text{eff}} = H^{(1)}_{\text{eff}}$.) The complete second-order reduced evolution operator \eqref{eq:169} then becomes

\begin{equation}
\bar{U}^{(2)}(0)P = \bar{U}^{(2)}(0)P + \frac{\delta U^{(1)}}{\delta E} \ast H^{(1)}_{\text{eff}}
\end{equation}

The result above is exact also for the quasi-degenerate case. The difference ratio can be expanded as discussed in Appendix 5

\begin{equation}
\frac{\delta U^{(1)}}{\delta E} = \frac{\partial U^{(1)}}{\partial E} + \frac{1}{2} \frac{\partial^2 U^{(1)}}{\partial^2 E} \delta E + \frac{1}{3!} \frac{\partial^3 U^{(1)}}{\partial^3 E} \delta E^2 + \cdots
\end{equation}

which in the limit of complete degeneracy yields

\begin{equation}
\bar{U}^{(2)}(0)P = \bar{U}^{(2)}(0)P + \frac{\partial U^{(1)}}{\partial E} \ast H^{(1)}_{\text{eff}}
\end{equation}
The second-order contribution to the wave operator (66) then becomes

\[
\Omega^{(2)}P = Q\tilde{U}^{(2)}(0)P = \tilde{\Omega}^{(2)}P + \frac{\delta \tilde{\Omega}^{(1)}}{\delta E} * H_{\text{eff}}^{(1)} \Rightarrow \tilde{\Omega}^{(2)}P + \frac{\delta \tilde{\Omega}^{(1)}}{\delta E} * H_{\text{eff}}^{(1)}
\]

(180)

where \(\tilde{\Omega}\) is the wave operator (90) without intermediate model space states.

The second-order contribution to the effective interaction is obtained by means of the relation (68). Since the expression (180) is valid only for \(t = 0\), it cannot be used to evaluate the time derivative. Instead, we have to use the original definition (168), and using the expressions (172) and (173), we find

\[
H_{\text{eff}}^{(2)} = PV(\mathcal{E}) \Gamma(\mathcal{E}) VP - PV(\mathcal{E})^\prime \Gamma(\mathcal{E}) V(\mathcal{E})P = \tilde{H}_{\text{eff}}^{(2)} + \frac{\delta \tilde{H}_{\text{eff}}^{(1)}}{\delta E} * H_{\text{eff}}^{(1)}
\]

(181)

where \(\tilde{H}_{\text{eff}}^{(2)} = PV\Gamma Q VP\) is the \(H - \text{bar}\) 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,

\[
H_{\text{eff}}^{(2)} = \tilde{H}_{\text{eff}}^{(2)} + \frac{\delta \tilde{H}_{\text{eff}}^{(1)}}{\delta E} * H_{\text{eff}}^{(1)} \Rightarrow \tilde{H}_{\text{eff}}^{(2)} + \frac{\delta \tilde{H}_{\text{eff}}^{(1)}}{\delta E} * H_{\text{eff}}^{(1)}
\]

(182)

4. Separable three-photon exchange

The treatment of the exchange of three separable covariant photons is quite analogous to the previous case. From the expansion (87) we have

\[
\tilde{U}^{(3)}P = \tilde{U}^{(3)}P + (\tilde{U}^{(2)} \tilde{P}\tilde{U}^{(1)}P - \tilde{U}^{(2)}P \cdot \tilde{U}^{(1)}P) + (\tilde{U}^{(1)} \tilde{P}\tilde{U}^{(2)}P - \tilde{U}^{(1)}P \cdot \tilde{U}^{(2)}P) + (\tilde{U}^{(1)} P\tilde{U}^{(1)}P - \tilde{U}^{(1)}P \cdot \tilde{U}^{(1)}P)(P\tilde{U}^{(1)}P - \cdot P\tilde{U}^{(1)}P)
\]

(183)

By generalizing the result of the preceding Appendix we obtain the relation

\[
AP BP - AP \cdot BP = \frac{\delta A}{\delta E} \cdot \tilde{B}
\]

(184)

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

\[
(\tilde{U}^{(2)} P\tilde{U}^{(1)}P - \tilde{U}^{(2)}P \cdot P\tilde{U}^{(1)}P) = \frac{\delta \tilde{U}^{(2)}}{\delta E} * P\tilde{U}^{(1)}P = \frac{\delta \tilde{U}^{(2)}}{\delta E} * \tilde{H}_{\text{eff}}^{(1)}
\]

(185)

\[
(\tilde{U}^{(1)} P\tilde{U}^{(2)}P - \tilde{U}^{(1)}P \cdot \tilde{U}^{(2)}P) = \frac{\delta \tilde{U}^{(1)}}{\delta E} * P\tilde{U}^{(2)}P = \frac{\delta \tilde{U}^{(1)}}{\delta E} * \tilde{H}_{\text{eff}}^{(2)}
\]

(186)

In the last term in Eq. (183) we have to apply the rule (184) twice, yielding

\[
(\tilde{U}^{(1)} P\tilde{U}^{(1)}P - \tilde{U}^{(1)}P \cdot \tilde{U}^{(1)}P)(P\tilde{U}^{(1)}P - \cdot P\tilde{U}^{(1)}P)
\]

\[
= \frac{\delta \tilde{U}^{(1)}}{\delta E} * P\tilde{U}^{(1)}P \cdot P\tilde{U}^{(1)}P = \frac{\delta \tilde{U}^{(1)}}{\delta E} \left(\frac{\delta \tilde{U}^{(1)}}{\delta E} * P\tilde{U}^{(1)}P\right) * P\tilde{U}^{(1)}P
\]

\[
= \frac{\delta}{\delta E} \left(\frac{\delta \tilde{U}^{(1)}}{\delta E} * \tilde{H}_{\text{eff}}^{(1)}\right) * \tilde{H}_{\text{eff}}^{(1)}
\]

(187)

From the previous Appendix (Eq. 178) we have

\[
\frac{\delta \tilde{U}^{(2)}}{\delta E} = \frac{\delta \tilde{U}^{(2)}}{\delta E} + \frac{\delta}{\delta E} \left(\frac{\delta \tilde{U}^{(1)}}{\delta E} * \tilde{H}_{\text{eff}}^{(1)}\right)
\]

(188)
and the complete result then becomes
\[ \tilde{U}^{(3)} P = \tilde{U}^{(3)} P + \frac{\delta \tilde{U}^{(2)}}{\delta \varepsilon} \frac{\delta H^{(1)}}{\delta \varepsilon} + \frac{\delta \tilde{U}^{(1)}}{\delta \varepsilon} \frac{\delta H^{(2)}}{\delta \varepsilon} \] (189)

This is an exact expression in this order, also for a quasi-degenerate model space. In the case of complete degeneracy this becomes
\[ \tilde{U}^{(3)} P = \tilde{U}^{(3)} P + \frac{\partial \tilde{U}^{(2)}}{\partial \varepsilon} \frac{\delta H^{(1)}}{\delta \varepsilon} + \frac{\partial \tilde{U}^{(1)}}{\partial \varepsilon} \frac{\delta H^{(2)}}{\delta \varepsilon} \] (190)

In terms of the \( \Omega \) operators the results above then become
\[ \Omega^{(3)} P = \overline{\Omega}^{(3)} P + \frac{\delta \Omega^{(2)}}{\delta \varepsilon} \frac{\delta \tilde{H}^{(1)}}{\delta \varepsilon} + \frac{\delta \Omega^{(1)}}{\delta \varepsilon} \frac{\delta \tilde{H}^{(2)}}{\delta \varepsilon} \] (191)

In order to obtain the third-order effective interaction, we consider the time derivative of the relation (183) (only the first factor is time dependent). This yields
\[ H^{(3)}_{\text{eff}} = \tilde{H}^{(3)}_{\text{eff}} + \frac{\delta \tilde{H}^{(1)}}{\delta \varepsilon} \tilde{H}^{(2)}_{\text{eff}} + \frac{\delta \tilde{H}^{(2)}}{\delta \varepsilon} \tilde{H}^{(1)}_{\text{eff}} + \frac{\delta \tilde{H}^{(1)}}{\delta \varepsilon} \frac{\delta \tilde{H}^{(1)}}{\delta \varepsilon} \tilde{H}^{(2)}_{\text{eff}} \] (192)

which using the relation (182) can be expressed
\[ \boxed{H^{(3)}_{\text{eff}} = \tilde{H}^{(3)}_{\text{eff}} + \frac{\delta \tilde{H}^{(1)}}{\delta \varepsilon} \tilde{H}^{(2)}_{\text{eff}} + \frac{\delta \tilde{H}^{(2)}}{\delta \varepsilon} \tilde{H}^{(1)}_{\text{eff}}} \] (193)

5. 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
\[ \frac{\delta f}{\delta x} = \delta_{x_0,x} f \frac{f(x) - f(x_0)}{x - x_0} \] (194)

which can be expanded in a Taylor series
\[ \frac{\delta f}{\delta x} = \delta_{x_0,x} f = f'(x_0) + \frac{1}{2} f''(x_0)(x-x_0) + \frac{1}{3!} f'''(x_0)(x-x_0)^2 + \frac{1}{4!} f^{IV}(x_0)(x-x_0)^3 + \cdots \] (195)

where
\[ f'(x_0) = \left. \frac{df}{dx} \right|_{x=x_0} \] (196)

etc.

Similarly, we define the second-order difference ratio
\[ \frac{\delta^2 f}{\delta^2 x} = \frac{\delta_{x^2,x} \delta_{x_0,x} f}{\delta x \delta x} = \frac{\delta_{x_0,x} f}{\delta x} \frac{\delta_{x_0,x} f}{\delta x} = \frac{1}{2} f''(x_0) + \frac{1}{3!} f'''(x_0)(x+x' - 2x_0) \]
\[ + \frac{1}{4!} f^{IV}(x_0) [(x-x_0)^2 + (x'-x_0)(x-x_0) + (x-x_0)^2] + \cdots \] (197)
the third-order difference ratio
\[ \frac{\delta^3 f}{\delta x^3} = \frac{\delta x''}{\delta x} \frac{\delta x - x'}{\delta x} \frac{\delta x' f}{\delta x} = \frac{1}{3!} f''''(x_0) + \frac{1}{4!} f^{IV}(x_0)(x + x' + x'' - 3x_0) + \cdots \] (198)

the fourth-order difference ratio
\[ \frac{\delta^4 f}{\delta x^4} = \frac{1}{4!} f^{IV}(x_0) + \cdots \] (199)

and so on.

Generalizing these results, we have in the limit, when the differences tend to zero
\[ \frac{\delta^n f}{\delta x^n} \Rightarrow \frac{1}{n!} \frac{d^n f}{d x^n} \] (200)

This relation is frequently used in the present paper.

References
1. E. E. Salpeter and H. A. Bethe, Phys. Rev. 84, 1232 (1951).
2. M. Gell-Mann and F. Low, Phys. Rev. 84, 350 (1951).
3. J. Schwinger, Proc. Nat. Acad. Sci. US 37, 452,455 (1951).
4. R. Karplus and A. Klein, Phys. Rev. 87, 848 (1952).
5. J. Schwinger, J. Math. Phys. 5, 1606 (1964).
6. J. M. Namyslowski, in Light-Front Quantization and Non-Perturbative QCD, J.P. Vary and F. Wolz, eds. (International Institute of Theoretical and Applied Physics, Ames) (1997).
7. F. J. Dyson, Phys. Rev. 91, 1543 (1953).
8. G. C. Wick, Phys. Rev. 96, 1124 (1953).
9. J. S. Goldstein, Phys. Rev. 91, 1516 (1953).
10. H. Sazdjian, J. Math. Phys. 28, 2618 (1987).
11. F. Gross, Phys. Rev. 186, 1448 (1969).
12. F. Gross, Phys. Rev. C 26, 2203 (1982).
13. I. T. Todorov, Phys. Rev. D 3, 2351 (1971).
14. W. E. Caswell and G. P. Lepage, Phys. Rev. A 18, 810 (1978).
15. J. H. Connell, Phys. Rev. D 43, 1393 (1991).
16. D. R. Phillips and S. J. Wallace, Phys. Rev. C 54, 507 (1996).
17. J. Bijtebier, Nucl. Phys. A 696, 581 (2001).
18. E. E. Salpeter, Phys. Rev. 87, 328 (1952).
19. W. Lucha, F. F. Schoberl, and D. Gromes, Physics Reports 200, 127 (1991).
20. A. Bender, C. D. Roberts, and L. vanSmekal, Phys. Lett. B 380, 7 (1996).
21. P. Maris and C. D. Roberts, Phys. Rev. C 56, 3369 (1997).
22. G. Onida, L. Reining, and A. Rubio, Rev. Mod. Phys. 74, 601 (2002).
23. N. E. Bickers, D. J. Scalapino, and S. R. White, Phys. Rev. Lett. 62, 961 (1989).
24. A. J. Williamson, C. J. Grossman, R. Q. Hood, A. Puzder, and G. Galli, Phys. Rev. Lett. 89, 196803 (2002).
25. V. C. Aguilera-Navarro, M. Fortes, and M. deLiano, Sol.State.Comm. 129, 577 (2004).
26. A. V. Kotikov and L. Lipatov, Nucl. Phys. B 661, 19 (2003).
27. A. M. Wang and T. N. Ruan, Comm. Theor. Phys. 33, 625 (2000).
28. J. G. Taylor, Phys. Rev. 150, 1321 (1966).
29. J. Bijtebier, Nucl. Phys. A 703, 327 (2002).
30. K. A. Brueckner, in The Many Body Theory, edited by C. DeWitt (Wiley and Sons, New York, 1959), p. 47.
31. A. L. Fetter and J. D. Walecka, The Quantum Mechanics of Many-Body Systems (McGraw-Hill, N.Y., 1971).
32. V. Pascualutsa and J. A. Tjon, Phys. Lett. B 435, 245 (1998).

NRC Canada
33. C. Schwartz and C. Zemach, Phys. Rev. 141, 1454 (1966).
34. W. B. Kaufmann, Phys. Rev. 187, 2051 (1969).
35. G. S. Adkins, R. N. Fell, and P. M. Mitrikov, Phys. Rev. A 65, 042103 (2002).
36. G. S. Adkins and R. N. Fell, Phys. Rev. A 60, 4461 (1999).
37. J. Sucher, Phys. Rev. 109, 1010 (1957).
38. J. Sucher, Ph.D. thesis, Columbia University, 1958, univ. Microfilm Internat., Ann Arbor, Michigan.
39. H. Araki, Prog. Theor. Phys. (Japan) 17, 619 (1957).
40. M. H. Douglas and N. M. Kroll, Ann. Phys. (N.Y.) 82, 89 (1974).
41. T. Zhang and G. W. F. Drake, J. Phys. B 27, L311 (1994).
42. T. Zhang and G. W. F. Drake, Phys. Rev. A 54, 4882 (1996).
43. T. Zhang, Phys. Rev. A 53, 3896 (1996).
44. T. Zhang, Phys. Rev. A 54, 1252 (1996).
45. G. W. F. Drake, Phys. Rev. A 19, 1387 (1979).
46. G. W. F. Drake, Can. J. Phys. 66, 586 (1988).
47. I. Lindgren and J. Morrison, Atomic Many-Body Theory (Second edition, Springer-Verlag, Berlin, 1986).
48. K. A. Brueckner, Phys. Rev. 100, 36 (1955).
49. J. Goldstone, Proc. R. Soc. London, Ser. A 239, 267 (1957).
50. B. H. Brandow, Rev. Mod. Phys. 39, 771 (1967).
51. F. Coster and H. Kümmer, Nucl. Phys. 17, 477 (1960).
52. J. Čižek, J. Chem. Phys. 45, 4256 (1966).
53. J. Paldus and J. Čižek, Adv. Quantum Chem. 9, 105 (1975).
54. R. J. Bartlett and G. D. Purvis, Int. J. Quantum Chem. 14, 561 (1978).
55. S. A. Kucharski and R. J. Bartlett, J. Chem. Phys. 97, 4682 (1992).
56. J. A. Pople, R. Krishnan, H. B. Schlegel, and J. S. Binkley, Int. J. Quantum Chem. 14, 545 (1978).
57. R. J. Bartlett, I. Shavitt, and G. D. Purvis, J. Chem. Phys. 71, 281 (1979).
58. I. Lindgren, J. Phys. B 7, 2441 (1974).
59. I. Lindgren, Int. J. Quantum Chem. S12, 33 (1978).
60. A.-M. Mårtensson-Pendrill, I. Lindgren, E. Lindroth, S. Salomonson, and D. S. Staudte, Phys. Rev. A 51, 3630 (1995).
61. P. J. Mohr, G. Plunien, and G. Soff, Physics Reports 293, 227 (1998).
62. Relativistic, Quantum Electrodynamic and Weak Interaction Effects in Atoms (AIP, ADDRESS, 1989), Vol. 189.
63. D. R. Plante, W. R. Johnson, and J. Sapirstein, Phys. Rev. A 49, 3519 (1994).
64. I. Lindgren, S. Salomonson, and B. Åsén, Physics Reports 389, 161 (2004).
65. I. Lindgren, Mol. Phys. 98, 1159 (2000).
66. I. Lindgren, B. Åsén, S. Salomonson, and A.-M. Mårtensson-Pendrill, Phys. Rev. A 64, 062505 (2001).
67. V. M. Shabaev, Physics Reports 356, 119 (2002).
68. V. Sauli and J. J. Adam, Phys. Rev. D 67, 085007 (2003).
69. C. Bloch, Nucl. Phys. 6, 329 (1958).
70. C. Bloch, Nucl. Phys. 7, 451 (1958).
71. S. S. Schweber, An Introduction to Relativistic Quantum Field Theory (Harper and Row, N.Y., 1961).
72. S. Blundell, P. J. Mohr, W. R. Johnson, and J. Sapirstein, Phys. Rev. A 48, 2615 (1993).
73. I. Lindgren, H. Persson, S. Salomonson, and L. Labzowsky, Phys. Rev. A 51, 1167 (1995).
74. D. Hedendahl, S. Salomonson, and I. Lindgren, (to appear).
75. A.-M. Mårtensson, J. Phys. B 12, 3995 (1980).
76. E. Lindroth, Phys. Rev. A 37, 316 (1988).
77. S. Salomonson and P. Öster, Phys. Rev. A 40, 5548 (1989).
78. S. Salomonson and P. Öster, Phys. Rev. A 40, 5559 (1989).