Chapter 1
Relativistically covariant many-body perturbation procedure

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Abstract

A covariant evolution operator (CEO) can be constructed, representing the time evolution of the relativistic wave function or state vector. Like the nonrelativistic version, it contains (quasi-)singularities. The regular part is referred to as the Green's operator, which is the operator analogue of the Green's function. This operator, which is a field-theoretical concept, is closely related to the many-body wave operator and effective Hamiltonian, and it is the basic tool for our unified theory. The Green's operator leads, when the perturbation is carried to all orders, to the Bethe-Salpeter equation (BSE) in the equal-time or effective-potential approximation. When relaxing the equal-time restriction, the procedure is fully compatible with the exact BSE. The calculations are performed in the photonic Fock space, where the number of photons is no longer constant. The procedure has been applied to heliumlike ions, and the results agree well with S-matrix results in cases when comparison can be performed. In addition, evaluation of higher-order QED-correlational effects has been performed, and the effects are found to be quite significant for light and medium-heavy ions.

1.1 Introduction

Relativistic covariance is an important concept in a relativistic theory. Well-known examples of covariant theories are Maxwell's theory of electromagnetism and Einstein's special theory of relativity. Many-body perturbation theories available today, on the other hand, are NOT relativistically covariant. A covariant many-body theory would, in principle, include electron correlation as well as quantum-electrodynamical effects (QED) to arbitrary order. In this paper such a procedure will be outlined. The first question is to what

extent this is an important problem, and where effects beyond the present procedures are expected to appear.

One important example is the study of *highly charged ions*, which are suitable objects for testing QED at very strong fields. With improved accelerators, particularly the new FAIR facility—*Facility for Antiproton and Ion Research*—now under construction at GSI in Darmstadt (see Fig. 1.1), new possibilities will appear to study transition energies (fine and hyperfine structure, Lamb shift), g-factors etc. with higher accuracy than was previously possible. In order to match the new experimental situation, it is important that also theoretical procedures are being developed. In the future *combined effects of QED and relativistic electron correlation* will be increasingly important—effects that presently cannot be evaluated.

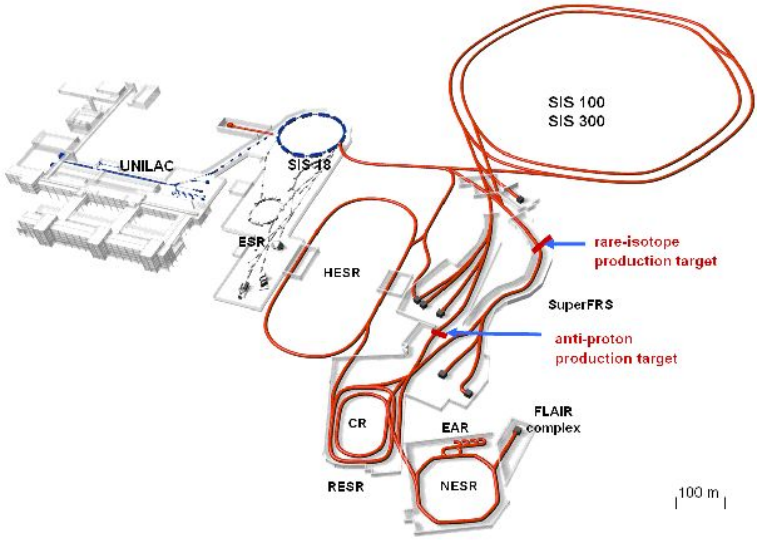

Fig. 1.1 FAIR project at GSI

Another example is the precision studies of light atoms and ions, such as the fine structure of the helium atom and heliumlike ions. Very accurate fine-structure separations have been determined for the helium atom and the Li^+ ion, but accurate results have also been achieved for somewhat heavier ions, like F^{+7} and Si^{+12} [1, 2]. For the helium atom there is a significant discrepancy between the experimental and theoretical results (see Fig. 1.2), the reason of which is presently unknown. The most accurate experimental results are obtained by Gabrielse [3] and by Inguscio et al. [4]. The theoretical calculations have been performed by Drake and coworkers [5] as well as by Pachucki and Sapirstein [6]. The theoretical calculations are based upon nonrelativistic wave functions of Hylleraas type with built-in electron correlation, while relativistic and QED effects are treated analytically in an $\alpha, Z\alpha$ power

expansion. Our aim is to develop a *numerical* procedure for calculating the *combined* relativistic, QED and correlation effects.

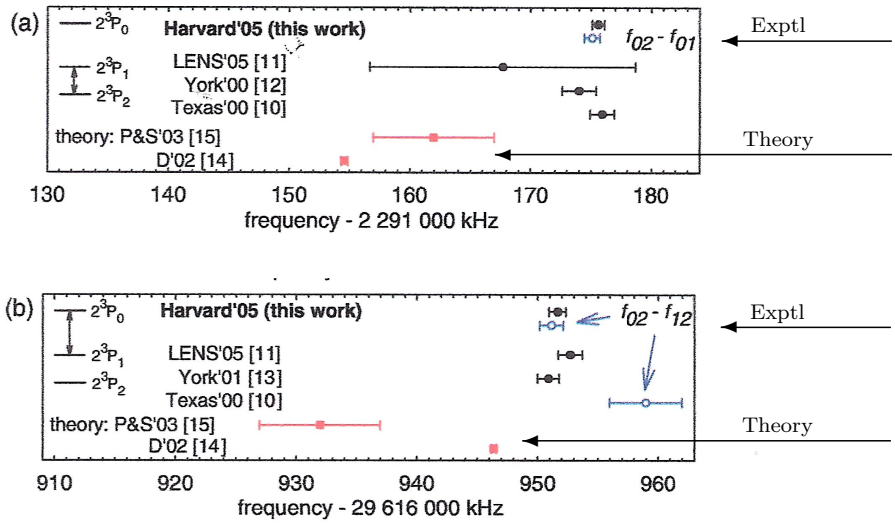

Fig. 1.2 Experimental and theoretical results for the fine-structure separations of the lowest P-state of the helium atom, $2^3P_1 - 2^3P_2$ top, $2^3P_0 - 2^3P_1$ bottom. (Picture taken from ref. [3].)

The many-body perturbative procedures are now well developed non-relativistically as well as relativistically [7]. Here, electron correlation can be treated essentially to all orders by methods of Coupled-Cluster type, while QED effects are at most included to first order. For pure QED calculations several methods have been developed. Most frequently used is the S-matrix formulation [8], which has been successfully applied particularly to highly charged ions. More recently, two other methods have been developed, the *Two-times Green's function technique* by Shabaev et al. [9], and the *Covariant Evolution Operator technique* (CEO), developed by the Göteborg group [10]. The latter two methods have the advantage over the S-matrix method that they can be applied to *quasi-degenerate states*, like fine-structure separations. As an illustration we consider the calculations performed by the Göteborg group a few years ago on some light heliumlike ions, compared with experimental data and the calculation by Drake et al. [11] (see Table 1.1). Our theoretical results agree with the experimental results within the assigned uncertainties, while some results of Drake fall outside the limits of error.

The methods for QED calculations presently available can for practical reasons only be applied to second order (two-photon exchange), which par-

ticularly for light systems yields an insufficient description of the electron correlation.

Table 1.1 Fine-structure separations for some heliumlike ions (from ref. [10])

Z	$^3P_1 - {}^3P_0$	$^3P_2 - {}^3P_0$	$^3P_2 - {}^3P_1$	
9	701(10) μH		4364,517(6)	Expt'l
	680	5050	4362(5)	Drake
	690	5050	4364	Göteborg
10	1361(6)	8455(6)	265880	Drake
	1370	8460	265880	Göteborg
18		124960(30)		Expt'l
		124810(60)		Drake
		124940		Göteborg

The CEO method has the advantage, compared to other techniques for QED calculations, that it has a structure quite similar to that of MBPT, which opens up the possibility of merging the two effects, as has been described in our recent publications [12, 13]. This will make it possible to develop for the first time a *relativistically MBPT procedure that is fully covariant*. Before going into this problem, we shall briefly summarize the standard time-independent and time-dependent perturbation procedures.

1.2 Time-independent perturbation procedure

1.2.1 Bloch equation

We assume that we have a set of *target states*, satisfying the non-relativistic Schrödinger equation

$$H\Psi^\alpha = E^\alpha \Psi^\alpha \quad (\alpha = 1, 2, ...d) \tag{1.1}$$

H is the Hamiltonian of the system[1]

$$H = \sum_{i=1}^{N} h_S(i) + \sum_{i<j}^{N} \frac{e^2}{4\pi r_{ij}} \tag{1.2}$$

where the first term is a sum of single-electron Schrödinger Hamiltonians and the second term represents the electrostatic interaction between the electrons.

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

For each target state we assume that there exists a *model state*, which in the *intermediate normalization* (IN) is the projection of the target state onto the *model space*

$$\Psi_0^\alpha = P\Psi^\alpha \tag{1.3}$$

Assuming the model states to be linearly independent, a *wave operator* transforms the model states back to the target states,

$$\Psi^\alpha = \Omega\Psi_0^\alpha \tag{1.4}$$

An *effective Hamiltonian* can be defined so that, operating entirely within the model space, it generates the exact energies of all the target states

$$H_{\text{eff}}\Psi_0^\alpha = E^\alpha\Psi_0^\alpha \tag{1.5}$$

In IN we have

$$H_{\text{eff}} = PH\Omega P \tag{1.6}$$

By partitioning the Hamiltonian into a model Hamiltonian (H_0) and a perturbation (V),

$$H = H_0 + V \tag{1.7}$$

the wave operator satisfies the *generalized Bloch equation* [14, 7]

$$\Big[\Omega, H_0\Big]P = \Big(V\Omega - \Omega V_{\text{eff}}\Big)P \tag{1.8}$$

Here,

$$V_{\text{eff}} = PV\Omega P \tag{1.9}$$

is the *effective interaction* and the effective Hamiltonian becomes

$$H_{\text{eff}} = PH_0P + V_{\text{eff}} \tag{1.10}$$

The Bloch equation (1.8) can be used to generate a perturbation expansion of Rayleigh-Schrödinger type also in the case of quasi-degeneracy by means of an extended model space. If the model space is *complete*, i.e. contains all configurations that can be formed by the valence electrons, then it can be shown that the expansion can be represented graphically by linked diagrams only, known as the *linked diagram* or *linked cluster theorem*,[2]

$$\Big[\Omega, H_0\Big]P = \Big(V\Omega - \Omega V_{\text{eff}}\Big)_{\text{linked}}P \tag{1.11}$$

By means of the *exponential Ansatz* $\Omega = \exp(T)$ the Bloch equation leads directly to the *Coupled-Cluster Approach*. For general open-shell systems it is often convenient to use the *normal-ordered exponential* [15]

[2] A *linked* diagram can consist of disconnected pieces, as long as they are all *open* in the sense that they do not operate entirely within the model space.

$$\Omega = \{\exp(T)\} \tag{1.12}$$

which eliminates unwanted contractions between the cluster operators. For a complete model space it then follows that the graphical representation of the expansion consists of *connected* diagrams only

$$\Big[T, H_0\Big]P = \Big(V\Omega - \Omega V_{\text{eff}}\Big)_{\text{conn}} P \tag{1.13}$$

Mukherjee has recently modified the normal-ordered exponential so that certain wanted contractions are maintained [16]

$$\Omega = \{\{\exp(T)\}\} \tag{1.14}$$

which improves the convergence in certain cases.

1.2.2 Perturbation expansion

As mentioned, the Bloch equation (1.8) is valid for arbitrary quasi-degenerate model spaces. For simplicity, though, we shall here illustrate how the expansion is performed for a degenerate model space (with energy E_0). We can then express the Bloch equation in the form

$$\Omega P = \Gamma_Q(E_0)\Big(V\Omega - \Omega V_{\text{eff}}\Big)P\,; \qquad \Gamma_Q(E_0) = \frac{Q}{E_0 - H_0} \tag{1.15}$$

which is essentially the original form of the equation, given by Bloch [17, 18]. In first order we have

$$\Omega^{(1)}P = \Gamma_Q(E_0)VP \tag{1.16}$$

and in second order

$$\Omega^{(2)}P = \Gamma_Q(E_0)\Big(V\Omega^{(1)} - \Omega^{(1)}V_{\text{eff}}^{(1)}\Big)P \tag{1.17}$$

where $V_{\text{eff}}^{(1)} = PVP$ is the first-order effective interaction. The second term is a so-called *folded term*, because it is traditionally drawn in a folded way (see Fig. 1.3), where the two parts can be evaluated independently. We shall see that this kind of effect plays an important role in the unified theory we are developing.

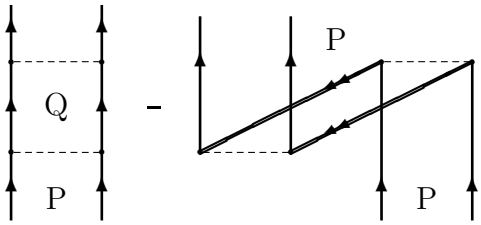

Fig. 1.3 Graphical representation of the second-order wave operator (1.17). The solid lines represent single-electron orbitals and the dashed lines instantaneous Coulomb interactions. The second folded diagram represents the part with the intermediate state in the model space (P).

1.2.3 Versions of MBPT/CCA

What is indicated here is a *multi-reference* approach, in which a multiple of states are treated simultaneously. This is particularly advantageous in calculating transitions energies. The *valence universal* version, valid for different stages of ionization, is particularly useful in evaluating ionization energies or electron affinities. A serious disadvantage with the multi-reference approach is that it often leads to so-called *intruder states*, i.e., states that do not belong to the group of target states under study but penetrate into the energy range of target states of the same symmetry when the perturbation is turned on. When this happens, the perturbation expansion no longer converges.

The effects of intruder states are generally more severe for molecules than for atoms, due to more dense energy levels. Therefore, even if there are ways of avoiding—or at least reducing—the effect of intruder states in the multi-reference approach, it is when the interest lies entirely in one or a few particular states, more advantageous to study one state at a time in a *state-specific approach* (see the paper by Paldus in this volume).

It is outside the scope of this paper to deal further with the various approaches of MBPT/CCA, which are well documented in the literature. Our main goal is to combine many-body calculations with QED, and here it is irrelevant exactly which many-body approach that is used.

1.2.4 Standard relativistic MBPT: QED effects

The standard relativistic MBPT procedures are based upon the *projected Dirac-Coulomb-Breit approximation* [19]

$$H = \Lambda_+ \Big[\sum_{i=1}^{N} h_D(i) + \sum_{i<j}^{N} \frac{e^2}{4\pi r_{ij}} + H_B \Big] \Lambda_+ \tag{1.18}$$

where h_D is the single-electron Dirac Hamiltonian and H_B is the instantaneous Breit interaction

$$H_B = -\frac{e^2}{8\pi} \sum_{i<j} \Big[\frac{\alpha_i \cdot \alpha_j}{r_{ij}} + \frac{(\alpha_i \cdot r_{ij})(\alpha_j \cdot r_{ij})}{r_{ij}^3} \Big] \tag{1.19}$$

Λ_+ is a projection operator that eliminates the negative-energy solutions of the Dirac equation. This approximation is also known as the *No-Virtual-Pair Approximation* (NVPA).

The diagrammatic representation of the NVPA for a two-electron system is exhibited in Fig. 1.4. The effects beyond the NVPA are traditionally referred to as *QED effects*, some of which are shown graphically in Fig. 1.5.

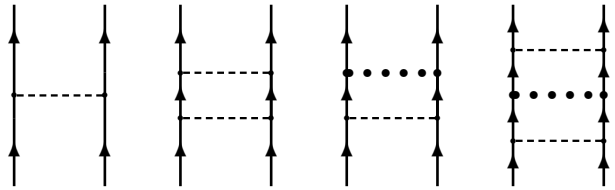

Fig. 1.4 Graphical representation of the NVPA for heliumlike systems. The dashed line represents, as before, the Coulomb interaction and the dotted line the instantaneous Breit interaction.

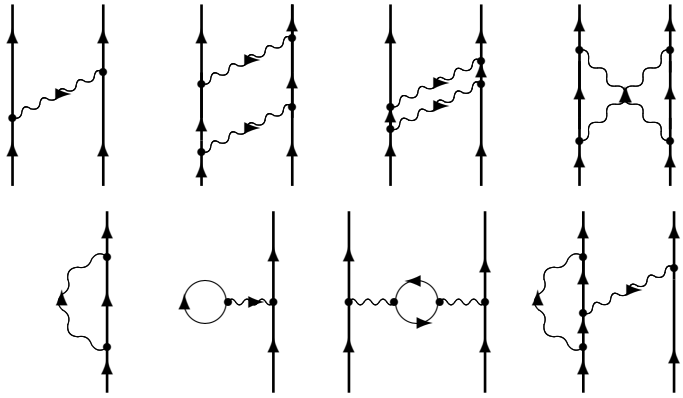

Fig. 1.5 Some low-order non-radiative (upper line) and radiative (lower line) "QED effects". The wavy lines represent the covariant photon exchange. These diagrams are *Feynman diagrams*, where the orbital lines can represent particle as well as hole or anti-particle states.

1.3 Time-dependent perturbation theory

1.3.1 Evolution operator

The time-dependent Schrödinger state vector has in the Schrödinger picture (SP) the time dependence

$$|\chi(t)\rangle = \mathrm{e}^{-\mathrm{i}H(t-t_0)}\,|\chi(t_0)\rangle \tag{1.20}$$

In the *interaction picture* (IP) the SP state vectors and operators are transformed according to

$$|\chi_{\mathrm{I}}(t)\rangle = \mathrm{e}^{\mathrm{i}H_0 t}\,|\chi_{\mathrm{S}}(t)\rangle; \qquad V_{\mathrm{I}}(t) = \mathrm{e}^{\mathrm{i}H_0 t}\,V\,\mathrm{e}^{-\mathrm{i}H_0 t} \tag{1.21}$$

This leads to the Schrödinger equation is in IP

$$\mathrm{i}\frac{\partial}{\partial t}|\chi_{\mathrm{I}}(t)\rangle = V_{\mathrm{I}}(t)\,|\chi_{\mathrm{I}}(t)\rangle \tag{1.22}$$

The *time-evolution operator* in IP, $U(t,t_0)$, is defined by[3]

$$|\chi(t)\rangle = U(t,t_0)\,|\chi(t_0)\rangle \qquad (t > t_0) \tag{1.23}$$

and it satisfies the differential equation

$$\mathrm{i}\frac{\partial}{\partial t}U(t,t_0) = V(t)\,U(t,t_0) \tag{1.24}$$

We assume that an *adiabatic damping* is applied

$$V(t) \to V(t)\,\mathrm{e}^{-\gamma|t|} \tag{1.25}$$

where γ is a small, positive number that eventually tends to zero. This leads to the expansion [20]

$$U_\gamma(t,t_0) = \sum_{n=0}^{\infty}\frac{(-\mathrm{i})^n}{n!}\int_{t_0}^{t}\mathrm{d}t_1\ldots\int_{t_0}^{t}\mathrm{d}t_n\,T\big[V(t_1)\ldots V(t_n)\big]\,\mathrm{e}^{-\gamma(|t_1|+|t_2|\ldots+|t_n|)} \tag{1.26}$$

where T is the *time-ordering operator*. The perturbation is represented by the interaction between an electron and the radiation fields

$$V(t) = \int \mathrm{d}^3x\,\mathcal{H}(t,\boldsymbol{x}) \tag{1.27}$$

with

[3] In the following we shall work mainly in the interaction picture and leave out the subscript "I".

$$\mathcal{H}(x) = -e\hat{\psi}(x)^\dagger \alpha^\mu A_\mu(x)\hat{\psi}(x) \tag{1.28}$$

where $x = (t, \boldsymbol{x})$ is the four-dimensional space-time coordinate and $\hat{\psi}(x)$, $\hat{\psi}(x)^\dagger$ and A_μ are the electron-field and the photon-field operators, respectively. This perturbation operates in the *extended photonic Fock space*, where the number of photons is no longer constant.[4] The expansion (1.26) then becomes

$$U(t,t_0) = \sum_{n=0}^{\infty} \frac{(-\mathrm{i})^n}{n!} \int_{t_0}^{t} \mathrm{d}x_1^4 \ldots \int_{t_0}^{t} \mathrm{d}x_n^4 \, T\big[\mathcal{H}(x_1)\ldots\mathcal{H}(x_n)\big] \, \mathrm{e}^{-\gamma(|t_1|+|t_2|\ldots+|t_n|)} \tag{1.29}$$

where the integrations are performed over all space and over time as indicated. The exchange of a single photon is represented by TWO perturbations of this kind.

1.3.2 Gell-Mann–Low theorem

Gell-Mann and Low [21] have shown that for a closed-shell system the state vector

$$|\chi(0)\rangle = |\Psi\rangle = \lim_{\gamma\to 0} \frac{U_\gamma(0,-\infty)|\Phi\rangle}{\langle\Phi|U_\gamma(0,-\infty)|\Phi\rangle} \tag{1.30}$$

satisfies the time-independent Schrödinger equation

$$(H_0 + V(0))|\Psi\rangle = E|\Psi\rangle \tag{1.31}$$

Here,

$$|\Phi\rangle = \lim_{t\to-\infty} |\chi(t)\rangle \tag{1.32}$$

is the *parent state*, equal to the limit of the time-dependent target function as the perturbation is adiabatically turned off. In the single-reference case this is identical to the model state (1.3). The Gell-Mann–Low (GML) theorem can be extended to a general open-shell system [10]

$$\boxed{\big|\chi^\alpha(0)\big\rangle = \big|\Psi^\alpha\big\rangle = \lim_{\gamma\to 0} \frac{N^\alpha \, U_\gamma(0,-\infty)\,\big|\Phi^\alpha\big\rangle}{\langle\Phi^\alpha|U_\gamma(0,-\infty)|\Phi^\alpha\rangle}} \tag{1.33}$$

In this case the parent state $|\Phi^\alpha\rangle$ is not necessarily identical to the model state, $|\Psi_0^\alpha\rangle = P|\Psi^\alpha\rangle$, which is the reason for the appearance of the normalization factor N^α. In this multi-reference case the wave functions satisfies similar equations

$$\boxed{(H_0 + V(0))|\Psi^\alpha\rangle = E^\alpha|\Psi^\alpha\rangle} \tag{1.34}$$

[4] Also the Fock space is a form of Hilbert space, and therefore we shall refer to the Hilbert space with a constant number of photons as the *restricted (Hilbert) space* and the space with a variable number of photons as the *extended or photonic Fock space*.

It should be observed that a condition for the GML relations to hold is that the *perturbation is time-independent in the Schrödinger picture*, apart from the adiabatic damping. With the Fock-space perturbation (1.27) this condition is fulfilled, but it is NOT true for any time-dependent perturbation, acting in the restricted space. Therefore, in the present formalism, which is based upon the GML theorem, *we have to work in the photonic Fock space.*

We can define a wave operator in the photonic space in the same way as before (1.4)

$$|\Psi^\alpha\rangle = \boldsymbol{\Omega}|\Psi_0^\alpha\rangle \tag{1.35}$$

(using bold-face symbol to distinguish it from the standard wave operator). From Eq. (1.34) we can also define a corresponding effective Hamiltonian

$$P\big(H_0 + V_{\text{eff}}\big)|\Psi_0^\alpha\rangle = E^\alpha|\Psi_0^\alpha\rangle \tag{1.36}$$

and

$$V_{\text{eff}} = PV(0)\boldsymbol{\Omega}P \tag{1.37}$$

Of course, the effective Hamiltonian/interaction lies in the model space, which is a part of the restricted Hilbert space with constant number of photons, while the wave operator now acts in the extended space.

1.4 Covariant evolution operator and the Green's operator

1.4.1 Definitions

The evolution operator (1.23) is a non-relativistic concept, since time evolves only in the positive direction. In relativistic applications we must allow time to run also *backwards* in the negative direction, which represents the propagation of *hole or antiparticle states* with negative energy. This leads to the *covariant evolution operator* (CEO), introduced by Lindgren, Salomonson and coworkers [10].

Here, we shall define the CEO by means of the *Green's function* (GF), using the Feynman kernel, which leads to relativistically covariance. The field-theoretical single-particle GF can be defined [22]

$$G(x, x_0) = \frac{\langle 0_{\text{H}}|T[\hat{\psi}_{\text{H}}(x)\hat{\psi}_{\text{H}}^\dagger(x_0)]|0_{\text{H}}\rangle}{\langle 0_{\text{H}}|\,0_{\text{H}}\rangle} \tag{1.38}$$

where T is the *Wick time-ordering* operator and $\hat{\psi}_{\text{H}}$, $\hat{\psi}_{\text{H}}^\dagger$ are the electron field operators in the Heisenberg representation. The state $|0_{\text{H}}\rangle$ is the *"Heisenberg vacuum"*. In the vacuum expectation all normal-ordered products vanish.

Therefore, in transforming the time-ordered product to normal ordering by means of Wick's theorem, only contractions will remain.

By transforming to the interaction picture, the vacuum expectation above can be expanded in analogy with the time evolution operator

$$\begin{aligned}\big\langle 0_{\rm H}\big|T[\hat\psi_{\rm H}(x)\hat\psi^\dagger_{\rm H}(x_0)]\big|0_{\rm H}\big\rangle &= \sum_{n=0}^{\infty}\frac{(-{\rm i})^n}{n!}\int\cdots\int {\rm d}t_1\cdots{\rm d}t_n\\ \times\langle 0|T\big[V(t_1)\cdots V(t_n)\;\hat\psi(x)\hat\psi^\dagger(x_0)\big]|0\rangle\;&{\rm e}^{-\gamma(|t_1|+|t_2|\cdots)}\end{aligned}\tag{1.39}$$

with *integrations over all times*. We now define the single-particle CEO[5]

$$U^1_{\rm Cov}(t,t_0)=\iint {\rm d}^3x\,{\rm d}^3x_0\;\hat\psi^\dagger(x)\big\langle 0_{\rm H}\big|T[\hat\psi_{\rm H}(x)\hat\psi^\dagger_{\rm H}(x_0)]\big|0_{\rm H}\big\rangle\;\hat\psi(x_0)\tag{1.40}$$

with integration over the space coordinates of x and x_0. This is obviously relativistically covariant.

The CEO is an *operator* in contrast to the GF, which is a *function*. In Fig. 1.6 we compare diagrams for single-photon exchange for the standard evolution operator, the GF and the CEO.

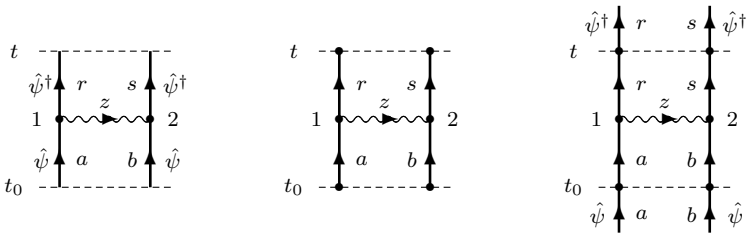

Fig. 1.6 Comparison between the standard evolution operator, the Green's function and the covariant evolution operator for single-photon exchange in the equal-time approximation. The solid lines between heavy dots represent electron propagators and the free lines electron creation and absorption operators.

The exchange of a single retarded photon is represented by *two* contracted perturbations of the type (1.27). The corresponding single-photon CEO can be shown to be [10][6]

$$\big\langle rs\big|U_{\rm sp}(t)\big|ab\big\rangle=\frac{{\rm e}^{-{\rm i}t(E_0-E_{\rm out})}}{E_0-E_{\rm out}}\,\langle rs|V_{\rm sp}(E_0)|ab\rangle\tag{1.41}$$

[5] In this definition we shall allow photons operators to remain uncontracted, for reasons that will be apparent later.

[6] When operating on unperturbed states with the adiabatic damping, the initial time is $t_0=-\infty$, which we normally leave out.

where V_{sp} is the effective single-photon potential

$$\langle rs|V_{\mathrm{sp}}(E_0)|ab\rangle = \Big\langle rs\Big|\int_0^\infty \mathrm{d}k\, f(k)\Big[\frac{1}{E_0-\varepsilon_r-\varepsilon_u-(k-\mathrm{i}\gamma)_r}+\frac{1}{E_0-\varepsilon_s-\varepsilon_t-(k-\mathrm{i}\gamma)_s}\Big]\Big|ab\Big\rangle \quad (1.42)$$

Here, ε_x represent the orbital energies and $E_0=\varepsilon_a+\varepsilon_b$ and $E_{\mathrm{out}}=\varepsilon_r+\varepsilon_s$ are the initial and final energies of the system, respectively. $(x)_r$ represents an expression with the sign of the orbital r, and $f(k)$ is a gauge-dependent function of the photon momentum. Note, that this potential depends on the initial energy, E_0.

1.4.2 Connection to MBPT

The vacuum expectation (1.39) contains singularities, which are eliminated by the denominator in the definition of the GF (1.38). For the CEO, which is an operator, the situation is more complex. We shall refer to the regular part of the CEO as the *Green's operator* (GO), which we separate into open and closed parts

$$\mathcal{G}(t,t_0)=1+\mathcal{G}_{\mathrm{op}}(t,t_0)+\mathcal{G}_{\mathrm{cl}}(t,t_0) \quad (1.43)$$

The open and closed parts of this operator are together identical to the previously introduced *reduced covariant evolution operator* $\widetilde{U}(t,t_0)$ [23, 10]

$$\widetilde{U}(t,t_0)=\mathcal{G}_{\mathrm{op}}(t,t_0)+\mathcal{G}_{\mathrm{cl}}(t,t_0) \quad (1.44)$$

The parts of the Green's operator are defined by

$$\begin{cases} QU(t,t_0)P=\mathcal{G}_{\mathrm{op}}(t,t_0)\cdot PU(0,t_0)P \\ PU(t,t_0)P=P+\mathcal{G}_{\mathrm{cl}}(t,t_0)\cdot PU(0,t_0)P \end{cases} \quad (1.45)$$

P is the projection operator for the model space and $Q=1-P$ for the complementary space. The *heavy dot* implies that the two parts are evaluated separately in the same way as in folded diagrams (Fig. 1.3).

It is easy to show that for $t=0$

$$U(0,t_0)P=\big(1+\mathcal{G}_{\mathrm{op}}(0,t_0)\big)\cdot PU(0,t_0)P \quad (1.46)$$

known as the *factorization theorem*. Inserting this into the GML formula (1.33), yields

$$|\Psi^\alpha\rangle_{\mathrm{Rel}}=\big(1+\mathcal{G}_{\mathrm{op}}(0,-\infty)\big)\cdot P\frac{N^\alpha\hat{U}_{\mathrm{Cov}}(0,-\infty)\big|\Phi^\alpha_{\mathrm{Rel}}\big\rangle}{\langle\Phi^\alpha_{\mathrm{Rel}}|\hat{U}_{\mathrm{Cov}}(0,-\infty)\,|\Phi^\alpha_{\mathrm{Rel}}\rangle} \quad (1.47)$$

The expression to the right of the dot is the model state $P|\Psi^\alpha\rangle_{\rm Rel} = |\Psi_0^\alpha\rangle_{\rm Rel}$, which implies that the expression to the left is the *relativistically covariant wave operator* (also a Fock-space operator)

$$\boxed{\boldsymbol{\Omega}_{\rm Cov} = 1 + \mathcal{G}_{\rm op}(0, -\infty)} \tag{1.48}$$

The *relativistically covariant effective interaction* can be shown to be [10]

$$\boxed{V_{\rm eff}^{\rm Cov} = P\Big(\mathrm{i}\frac{\partial}{\partial t}\,\mathcal{G}_{\rm cl}(t, -\infty)\Big)_{t=0} P} \tag{1.49}$$

1.4.3 Model-space contributions

In the definition of the Green's function (1.38) the singularities of the vacuum expectation appear only in the form of disconnected diagrams. For the Green's operator, on the other hand, (quasi-)singularities can appear also for connected diagrams, when an intermediate state lies in the model space. We shall consider here two-electron systems, and we shall see how these singularities can be eliminated.

From the definitions (1.45) of the Green's operator it follows that the open part can be expanded as

$$\mathcal{G}_{\rm op}(t)P = U_{\rm op}(t)P - \mathcal{G}_{\rm op}(t)\cdot\mathcal{G}_{\rm cl}(0)P - \mathcal{G}_{\rm op}(t)\cdot\mathcal{G}_{\rm cl}(0)\cdot\mathcal{G}_{\rm cl}(0)P - \cdots \tag{1.50}$$

The negative terms are referred to as *counterterms*, which eliminate the (quasi-)singularities of the CEO, $U_{\rm op}$.

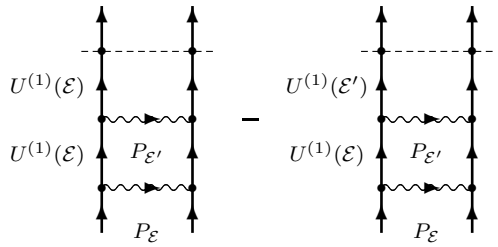

Fig. 1.7 Elimination of singularity of the second-order evolution operator by means of a counterterm (second diagram).

We consider a ladder diagram with two photons, shown in Fig. 1.7 (left), and we assume that we operate on a model-space state of energy $\mathcal{E}$. (We recall that the perturbation in this formalism is the interaction (1.27), which implies that each retarded photon exchange is a second-order perturbation.)

For the single photon we have for $t = 0$

$$\mathcal{G}^{(1)}(\mathcal{E})P_{\mathcal{E}} = U_{\rm sp}^{(1)}(\mathcal{E})P_{\mathcal{E}} = \mathit{\Gamma}_{\mathcal{E}}\, V_{\rm sp}(\mathcal{E})P_{\mathcal{E}} = \frac{1}{\mathcal{E}-H_0}\, V_{\rm sp}(\mathcal{E})P_{\mathcal{E}} \tag{1.51}$$

where $V_{\rm sp}(\mathcal{E})$ is the energy-dependent single-photon potential (1.42). (Also the evolution operator and the Green's operator depend on the energy to the right, which we have indicated, leaving out the time.) The two-photon CEO can be expressed as a product of two single-photon CEOs, both with the same energy parameter $\mathcal{E}$,

$$U_{\rm sp}^{(2)}(\mathcal{E})_{\rm Ladd}P_{\mathcal{E}} = U_{\rm sp}^{(1)}(\mathcal{E})\, U_{\rm sp}^{(1)}(\mathcal{E})\, P_{\mathcal{E}} = \frac{1}{\mathcal{E}-H_0}\, V_{\rm sp}(\mathcal{E})\frac{1}{\mathcal{E}-H_0}\, V_{\rm sp}(\mathcal{E})P_{\mathcal{E}} \tag{1.52}$$

We assume now that we have an intermediate model-space state of energy $\mathcal{E}' \approx \mathcal{E}$, which makes the expression quasi-singular,

$$\begin{aligned} U_{\rm sp}^{(2)}(\mathcal{E})_{\rm Ladd}P_{\mathcal{E}} &= U_{\rm sp}^{(1)}(\mathcal{E})\, P_{\mathcal{E}'}\, U_{\rm sp}^{(1)}(\mathcal{E})\, P_{\mathcal{E}} = \frac{1}{\mathcal{E}-H_0}\, V_{\rm sp}(\mathcal{E})\frac{P_{\mathcal{E}'}}{\mathcal{E}-H_0}\, V_{\rm sp}(\mathcal{E})P_{\mathcal{E}} \\ &= U_{\rm sp}^{(1)}(\mathcal{E})\, \frac{1}{\mathcal{E}-\mathcal{E}'}\, P_{\mathcal{E}'}V_{\rm sp}(\mathcal{E})P_{\mathcal{E}} \end{aligned} \tag{1.53}$$

Here, $P_{\mathcal{E}'}V_{\rm sp}(\mathcal{E})P_{\mathcal{E}}$ is the single-photon effective interaction, which is identical to the second-order effective interaction (1.37) with the Fock-space wave operator.

The counterterm looks similar, but the second factor has the energy parameter $\mathcal{E}'$ (it does not operate beyond the heavy dot)

$$\begin{aligned} U_{\rm sp}^{(2)}(\mathcal{E})_{\rm Counter}P_{\mathcal{E}} &= -U_{\rm sp}^{(1)}(\mathcal{E}')P_{\mathcal{E}'} \cdot P_{\mathcal{E}'}U_{\rm sp}^{(1)}(\mathcal{E})\, P_{\mathcal{E}} \\ &= -U_{\rm sp}^{(1)}(\mathcal{E}')\, \frac{P_{\mathcal{E}'}}{\mathcal{E}-\mathcal{E}'}\, V_{\rm sp}(\mathcal{E})P_{\mathcal{E}} \end{aligned} \tag{1.54}$$

This eliminates the (quasi-)singularity, but there is a finite remainder,

$$\frac{U_{\rm sp}^{(1)}(\mathcal{E}) - U_{\rm sp}^{(1)}(\mathcal{E}')}{\mathcal{E}-\mathcal{E}'}\, P_{\mathcal{E}'}V_{\rm sp}(\mathcal{E})P_{\mathcal{E}} = \frac{\delta U_{\rm sp}^{(1)}(\mathcal{E})}{\delta\mathcal{E}}\, V_{\rm eff}^{(1)} \Rightarrow \frac{\partial U_{\rm sp}^{(1)}(\mathcal{E})}{\partial\mathcal{E}}\, V_{\rm eff}^{(1)} \tag{1.55}$$

Differentiating the single-photon CEO, we find that the two-photon Green's operator becomes

$$\mathcal{G}(\mathcal{E})^{(2)}P_{\mathcal{E}} = \mathit{\Gamma}_{\mathcal{E}}\Big(V_{\rm sp}(\mathcal{E})\, \Omega^{(1)} - \Omega^{(1)}V_{\rm eff}^{(1)} + \frac{\delta V_{\rm sp}(\mathcal{E})}{\delta\mathcal{E}}\, V_{\rm eff}^{(1)}\Big)P_{\mathcal{E}} \tag{1.56}$$

where $\mathit{\Gamma}_{\mathcal{E}}$ is defined in Eq. (1.51). The last two terms are due to the intermediate model-space state, and we refer to them as the *model-space contribution* (MSC). This is quite analogous to the folded term in Eq. (1.17) in standard MBPT, the only difference being that we now have an additional term, due to the energy dependence of the perturbation.

We have so far only considered multiple single-photon exchange, but this can be generalized to the full exchange of irreducible interactions, $\mathcal{V}(\mathcal{E})$, shown in Fig. 1.8, yielding

$$\mathcal{G}(\mathcal{E})^{(2)}P_{\mathcal{E}} = \mathit{\Gamma}_{\mathcal{E}}\Big(\mathcal{V}(\mathcal{E})\,\Omega^{(1)} - \Omega^{(1)}V_{\text{eff}}^{(1)} + \frac{\delta\mathcal{V}(\mathcal{E})}{\delta\mathcal{E}}\,V_{\text{eff}}^{(1)}\Big)P_{\mathcal{E}} \tag{1.57}$$

where we now have

$$V_{\text{eff}} = P\mathcal{V}(\mathcal{E})\Omega P \tag{1.58}$$

with the operators acting in the restricted space.

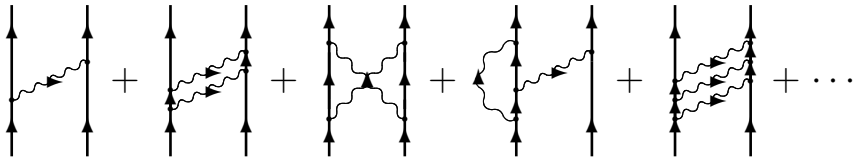

Fig. 1.8 Irreducible potential interactions, acting in the restricted space.

1.5 Connection to Bethe-Salpeter equation

1.5.1 Equal-time approximation

When the procedure of the previous section is continued, one finds that the Green's operator can be expended as [12, 13]

$$\mathcal{G}(\mathcal{E}) = \mathcal{G}_0(\mathcal{E}) + \sum_{n=1}^{\infty}\frac{\delta^n\mathcal{G}_0(\mathcal{E})}{\delta\mathcal{E}^n}\left(V_{\text{eff}}\right)^n \tag{1.59}$$

where $\mathcal{G}_0(\mathcal{E})$ represents the Green's operator without any intermediate model-space states (no folds). It then follows that the second term of the expansion represents the entire MSC.

When we operate with the expansion (1.59) on the model state $|\Phi\rangle$ with energy E_0, the result is

$$\mathcal{G}(E_0)\big|\Phi\big\rangle = \Big[\mathcal{G}_0(\mathcal{E}) + \sum_{n=1}^{\infty}\frac{\delta^n\mathcal{G}_0(\mathcal{E})}{\delta\mathcal{E}^n}\left(\mathit{\Delta}E\right)^n\Big]_{\mathcal{E}=E_0}\big|\Phi\big\rangle \tag{1.60}$$

The effective interaction (1.58) with the full irreducible potential and with the wave operator in the restricted Hilbert space is also equal to $V_{\rm eff} = PV(0)\boldsymbol{\Omega}P$ with the interaction (1.27) and the Fock-space wave operator. Therefore, according to Eq. (1.36),

$$V_{\rm eff}|\Phi\rangle = (E - E_0)|\Phi\rangle = \Delta E|\Phi\rangle \tag{1.61}$$

This is a Taylor series, and the result can be expressed

$$\mathcal{G}(E_0)\big|\Phi\big\rangle = \mathcal{G}_0(E)\big|\Phi\big\rangle \tag{1.62}$$

This implies that *the effect of the model-space contributions is to shift the energy parameter from the model energy E_0 to the target energy E.*

From

$$\mathcal{G}_0(E_0) = 1 + \Big[\frac{1}{E_0 - H_0}\,\mathcal{V}(E_0) + \frac{1}{E_0 - H_0}\,\mathcal{V}(E_0)\frac{Q}{E_0 - H_0}\,\mathcal{V}(E_0) + \cdots\Big] \tag{1.63}$$

we then find that the Green's operator *with* MSC becomes

$$\mathcal{G}(E_0) = \mathcal{G}_0(E) = 1 + \Big[\frac{1}{E - H_0}\,\mathcal{V}(E) + \frac{1}{E - H_0}\,\mathcal{V}(E)\frac{Q}{E - H_0}\,\mathcal{V}(E) + \cdots\Big] \tag{1.64}$$

The open part of the Green's operator represents the open part of the wave operator (1.48), i.e.,

$$Q\Psi = \Big[\frac{Q}{E - H_0}\,\mathcal{V}(E) + \frac{Q}{E - H_0}\,\mathcal{V}(E)\frac{Q}{E - H_0}\,\mathcal{V}(E) + \cdots\Big]|\Phi\rangle \tag{1.65}$$

or

$$Q(E - H_0)\,\Psi = Q\mathcal{V}(E)\,\Psi \tag{1.66}$$

From Eq. (1.61) we have

$$P(E - H_0)|\Psi\rangle = V_{\rm eff}(E)|\Phi\rangle = P\mathcal{V}(E)\Psi \tag{1.67}$$

which yields

$$\boxed{(E - H_0)|\Psi\rangle = \mathcal{V}(E)|\Psi\rangle} \tag{1.68}$$

This is the ***Bethe-Salpeter equation in the effective-potential form***. We can regard this equation as the projection of the Fock-space equation (1.34) onto the restricted space.

We have here assumed that the CEO represents the time evolution of the relativistic wave function (1.23), which has the consequence that it depends only on a single initial and a single final time, the same for all particles. In the next section we shall relax this restriction and let the times be independent for the individual particles. Then we will retrieve the exact Bethe-Salpeter equation. This leads to a manifestly covariant concept, although it is not in accord with standard quantum mechanics.

1.5.2 The full Bethe-Salpeter equation

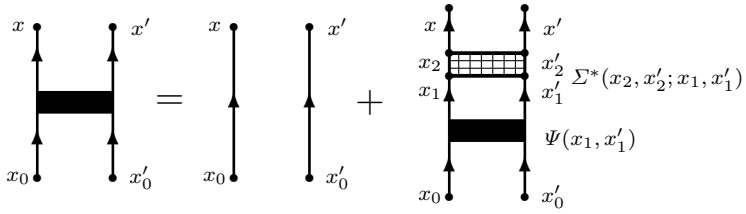

Fig. 1.9 Graphical representation of the Dyson equation for the two-particle Green's function. The crossed box represents the proper or irreducible two-particle self energy.

The Dyson equation for the two-particle Green's function, illustrated in Fig. 1.9, can be expressed

$$G(x,x';x_0,x_0') = G_0(x,x';x_0,x_0') + \iiiint \mathrm{d}^4x_1\mathrm{d}^4x_2\mathrm{d}^4x_1'\mathrm{d}^4x_2' \times G_0(x,x';x_2,x_2')\,(-\mathrm{i})\Sigma^*(x_2,x_2';x_1,x_1')\,G(x_1,x_1';x_0,x_0') \tag{1.69}$$

where Σ^* is the *proper* or *irreducible* two-particle self energy (that cannot be separated into two or more self-energy parts). G_0 is the zeroth-order two-particle Green's function, which can also be "dressed" with single-particle self-energy insertions.

Bethe and Salpeter [24] as well as Gell-Mann and Low [21] argue that a similar equation can be set up for a two-particle wave function. We assume we have a single-reference situation and let the Dyson equation act on the unperturbed wave function of model function $\Phi(x_0,x_0')$ (with $t_0 = t_0' = -\infty$) . With

$$\Psi(x,x') = \iint \mathrm{d}^3x_0\mathrm{d}^3x_0'\,G(x,x';x_0,x_0')\,\Phi(x_0,x_0') \tag{1.70}$$

and

$$\Phi(x,x') = \iint \mathrm{d}^3x_0\mathrm{d}^3x_0'\,G_0(x,x';x_0,x_0')\,\Phi(x_0,x_0') \tag{1.71}$$

we have

$$\boxed{\Psi(x,x') = \Phi(x,x') + \iiiint \mathrm{d}^4x_1\mathrm{d}^4x_2\mathrm{d}^4x_1'\mathrm{d}^4x_2' \times G_0(x,x';x_2,x_2')\,(-\mathrm{i})\Sigma^*(x_2,x_2';x_1,x_1')\,\Psi(x_1,x_1')} \tag{1.72}$$

This is the famous *Bethe-Salpeter equation*, which is illustrated graphically in Fig. 1.10. In the treatment of Bethe–Salpeter and Gell-Mann–Low free-electron propagators are used, and then the first inhomogeneous term cannot

contribute to a bound state. Here, we shall work in the Ferry picture with bound-state propagators, and then this term should remain.

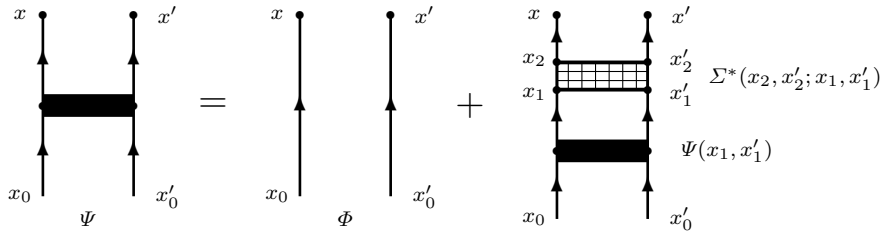

Fig. 1.10 Graphical representation of the *inhomogeneous* Bethe-Salpeter equation (1.72). This is similar to Fig. 1.9 but operates now on the unperturbed wave function.

By means of the two-times Green's operator Eq. (1.70) can be expressed as an operator relation

$$\boxed{|\Psi(t,t')\rangle = \mathcal{G}(t,t';-\infty)\,|\Phi\rangle} \tag{1.73}$$

which implies that *the two-times Green's operator* essentially represents wave operator of the Bethe-Salpeter state vector. It also follows that the *the four-times Green's operator* acts as a time-evolution operator of the two-times Green's function

$$\boxed{|\Psi(t,t')\rangle = \mathcal{G}(t,t';t_0,t'_0)\,|\Psi(t_0,t'_0)\rangle} \tag{1.74}$$

1.6 Implementation

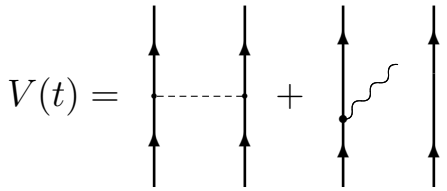

Fig. 1.11 Graphical representation of the perturbation (1.78), acting in the photonic Fock space.

In order to implement the procedure developed above, it is convenient to work in the photonic Fock space, where the number of photons is no longer constant.

We consider for simplicity the single-reference case and start with the Fock-space relation (1.34) and the corresponding Fock-space Bloch equation

$$\Big[\boldsymbol{\Omega}, H_0\Big] P = \Big(V(0)\boldsymbol{\Omega} - \boldsymbol{\Omega} V_{\text{eff}}\Big) P \tag{1.75}$$

We use here the Coulomb gauge, where the interaction can be separated in an instantaneous Coulomb part and a Breit interaction that can be retarded. The Breit part is represented by two interactions of the type (1.27) with the $f(k)$ function in Eq. (1.42) given by

$$f_{\text{C}}(k) = \boldsymbol{\alpha_1} \cdot \boldsymbol{\alpha_2} \, \frac{\sin(kr_{12})}{\pi r_{12}} - (\boldsymbol{\alpha_1} \cdot \boldsymbol{\nabla_1}) \, (\boldsymbol{\alpha_2} \cdot \boldsymbol{\nabla_2}) \, \frac{\sin(kr_{12})}{\pi k^2 \, r_{12}} \tag{1.76}$$

where the nabla operators do not operate beyond the factor shown. The terms here represent the Gaunt and scaler-retardation parts of the interaction, respectively.

The function $f_{\text{C}}(k)$ can be expanded in partial waves

$$f_{\text{C}}(k) = \sum_{l=0}^{\infty} \Big[V_G^l(kr_1) \cdot V_G^l(kr_2) - V_{\text{sr}}^l(kr_1) \cdot V_{\text{sr}}^l(kr_2) \Big] \tag{1.77}$$

In the photonic Fock space the perturbation is then of the form

$$V = V_{\text{C}} + V_{\text{G}}^l(kr) + V_{\text{sr}}^l(kr) \tag{1.78}$$

which is time independent. This is illustrated in Fig. 1.11. Applying this simple perturbation in the Fock space is equivalent to applying the complicated perturbation in Fig. 1.8 in the restricted space.

The photonic-Fock-space Bloch equation now becomes

$$\big[\boldsymbol{\Omega}, H_0\big] P = \big(V_{\text{C}} + V_1^l + V_2^l\big) \, \boldsymbol{\Omega} P - \boldsymbol{\Omega} V_{\text{eff}} \tag{1.79}$$

letting V^l represent the Gaunt term as well as the scalar retardation. Applying, for instance, first a series of Coulomb interactions, then a perturbation V^l, then a new series of Coulomb interactions, a second V^l perturbation and finally a new series of Coulomb interactions, leads to the result shown in Fig. 1.12. This represents a single time-dependent photon with crossing Coulomb interactions, evaluated with correlated wave function. In addition, folded diagrams have to be included, which also represent the energy derivatives (1.56). By closing the photon on the same electron line, corresponding self-energy and vertex correction effects are obtained (of course, after proper renormalization).

The procedure presented here has been applied to a number of light and medium-heavy heliumlike ions, and the results agree well with standard S-matrix results in cases where comparison can be made. In addition, effects of single retarded photon with correlation—with and without crossing Coulomb interactions—have been evaluated and found to yield effects that are quite significant and more important than second-order QED effects for light elements. More details about the implementation procedure and numerical results will appear in a forthcoming publication.

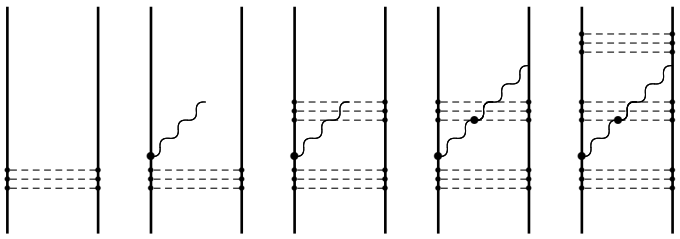

Fig. 1.12 Graphical representation of the perturbative solution of the Fock-space Bloch equation (1.79).

1.7 Summary and conclusions

We have presented a relativistically covariant many-body perturbation procedure, based upon the covariant evolution operator and the Green's operator. This represents a unification of the many-body perturbation theory and quantum-electrodynamics. Applied to all orders, the procedure leads in the equal-time approximation to the Bethe-Salpeter equation (BSE) in the effective-potential form. By relaxing this restriction, the procedure is consistent with the full BSE. The new procedure will be of importance in cases where QED effects beyond first order in combination with high-order electron correlation is significant.

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