

Many-body procedure for energy-dependent perturbation: Merging many-body perturbation theory with QED

Ingvar Lindgren,^{*} Sten Salomonson,[†] and Daniel Hedendahl[‡]
Physics Department, Göteborg University, Göteborg, Sweden

(Received 7 February 2006; published 7 June 2006)

A formalism for energy-dependent many-body perturbation theory (MBPT), previously indicated in our recent review articles [Lindgren *et al.*, Phys. Rep. **389**, 161 (2004); Can. J. Phys. **83**, 183 (2005)], is developed in more detail. The formalism allows for an arbitrary mixture of energy-dependent (retarded) and energy-independent (instantaneous) interactions and hence for a merger of quantum-electrodynamics (QED) and standard (relativistic) MBPT. This combined many-body-QED procedure is particularly important for light elements, such as light heliumlike ions, where electron correlation is pronounced. It can also be quite significant in the medium-heavy mass range, as recently discussed by Fritzsche *et al.* [J. Phys. B **38**, S707 (2005)], with the consequence that the effects might be significant also in analyzing the data of experiments with highly charged ions. A numerical procedure is described, and some preliminary results are given for heliumlike ions with a single retarded photon. This represents the first numerical evaluation of the combined many-body-QED effect on an atomic system. It is found that for heliumlike neon the effect of one retarded photon with correlation represents more than 99% of the nonradiative effects beyond energy-independent MBPT. The new procedure also allows for the inclusion of radiative effects (self-energy and vacuum polarization) in a more systematic fashion than has previously been possible.

DOI: [10.1103/PhysRevA.73.062502](https://doi.org/10.1103/PhysRevA.73.062502)

PACS number(s): 31.15.Md, 31.30.Jv

I. INTRODUCTION

What is commonly known as many-body perturbation theory (MBPT) is a class of perturbative schemes for bound atomic, molecular or nuclear states with a time- or energy-independent perturbation, based upon the Rayleigh-Schrödinger perturbative scheme, such as the Brueckner-Goldstone linked-diagram expansion or variants thereof [1]. Also certain iterative or “all-order” approaches, like the coupled-cluster approach (CCA) or “Exponential Ansatz,” can be referred to this category, although they are not strictly perturbative in nature. All these approaches can in principle treat the electron correlation to arbitrary order. In addition, they have—as distinct from procedures based upon the Brillouin-Wigner (BW) perturbation expansion—the important property of being *size extensive* in the sense that the energy scales linearly with the size of the system. Furthermore, by using an extended or multi-reference model space such schemes can also successfully handle the *quasidegenerate* problem with closely spaced energy levels that are strongly mixed by the perturbation.

For time- or energy-dependent perturbations, like those of quantum-electrodynamics (QED), the situation is quite different and much less developed. There is presently no numerical scheme available that can treat energy-dependent perturbations together with electron correlation to arbitrary order, and also the treatment of quasidegeneracy forms a serious problem in connection with such interactions. In the numerical methods presently available for QED calculations the electron-electron interaction is treated by the exchange of

fully covariant photons, which is quite a tedious—and usually unnecessarily tedious—process to handle the electron correlation. At most two-photon exchange can be treated in this way with computers available today, which is insufficient for light and medium-heavy elements, where the electron correlation can be quite important.

A major problem in extending the energy-dependent perturbation theory to include electron correlation is that most methods have a structure that is quite different from that of energy-independent perturbation theory, which makes it difficult to utilize the well-developed methods of the latter. Of the available methods only the *covariant evolution operator* (CEO) method, that we recently developed, has a structure that is akin to standard energy-independent MBPT [2–4]. This opens the possibility of combining the two approaches into a *many-body-QED procedure*, as proposed in our recent review articles [4,5] and further developed in the present work. In that scheme the CEO method is combined with all-order MBPT methods of coupled-cluster type, so that the exchange of covariant photons can be mixed with an arbitrary number of instantaneous Coulomb interactions. In this way electron correlation can, for the first time, be treated to arbitrary order together with energy-dependent interactions of QED type.

The retarded electron-electron interaction can be treated in an approximate way by means of the so-called Mittleman approximation [6–9]. This potential, however, is originally based upon energy conservation and, therefore, yields the correct result only in first order (see, for instance, Eq. (300) of Ref. [4]). In higher orders it is doubtful if it leads to better results than the simple unretarded Breit interaction (see, for instance [10], p. 1188).

The CEO method was originally developed in order to be able to treat the quasidegeneracy problem in QED calculations. The standard procedure for bound-state QED is the

^{*}Email address: ingvar.lindgren@fy.chalmers.se

[†]Email address: f3asos@fy.chalmers.se

[‡]Email address: dahe@fy.chalmers.se

S -matrix formulation [11], which has been successfully applied particularly to highly charged ions. For lighter elements—in addition to the electron-correlation problem—also the quasidegeneracy problem might be quite pronounced, and the S -matrix formulation fails. One illustrative example is the fine structure of heliumlike ions, where in the relativistic formulation, for instance, the lowest triplet state 3P_1 is a mixture of the basis states $1s2p_{1/2}$ and $1s2p_{3/2}$, which are very closely spaced in energy and strongly mixed for light elements. In order to be able to use the procedure of standard MBPT, where quasidegenerate states are included in an extended model space, off-diagonal elements of the effective Hamiltonian have to be evaluated, which is not possible in the standard S -matrix formulation, due to the energy conservation of the scattering process [12]. In the CEO method, based upon the evolution operator for *finite* time [4], the extended-model-space technique can be used, and a few years ago we applied this to evaluate QED contributions to the fine structure for heliumlike ions, including the quasidegenerate 3P_1 state, down to $Z=9$ [3]. The same problem has very recently been treated by Shabaev *et al.* down to $Z=12$, using the *two-times Green's function technique* [13–15]. Furthermore, the presently available methods for numerical QED calculations suffer from the shortcoming that they are not applicable to the lightest elements—below $Z=10$, say—due to convergence problems. The extension of the CEO method to include electron correlation to arbitrary order, presented here, is expected to remedy this problem.

The most accurate calculations on light heliumlike ions have been performed by the analytical or “unified” method of Drake and related techniques [16–20]. This is based upon expansion in powers of the fine-structure constant α of the Bethe-Salpeter equation and the Brillouin-Wigner (BW) perturbation series [21,22]. It leads to an extremely high accuracy for the lightest elements, but being based upon the BW perturbation expansion, the procedure is *not* size-extensive and less suitable for larger systems.

From a comparison between theoretical calculations and experiments [23–25] on the helium fine structure, a value of the fine-structure constant can in principle be deduced. There is presently, however, a discrepancy of about five standard deviations between the value deduced in this way and the established value based upon the $g-2$ value of the electron, used in the CODATA adjustment [26]. Hopefully, the technique presented here could in the future—in combination with analytical calculations—contribute to a more accurate theoretical fine-structure evaluation and in this way resolve the present discrepancy.

In addition to the light heliumlike ions and other light systems, the combination of QED and many-body effects can be of importance also for heavier systems, as recently discussed by Fritzsche *et al.* [27]. They have analyzed this problem particularly with regard to possible heavy-ion experiments of the type that can be performed at the big storage rings, like that at GSI in Darmstadt. They then conclude that the accurate treatment of the interplay between QED and many-body effects constitutes one of the most challenging problems in connection with highly charged-ion experiments.

The present paper will be organized as follows. In the next section we briefly review the standard perturbation

theory for time-independent and time-dependent perturbations, and next we summarize the properties of our recently introduced covariant evolution-operator method. The following main section deals with the development of the numerical many-body-QED method by deriving Bloch equations for combined retarded and instantaneous interactions. Finally, we describe briefly our numerical procedure and give some preliminary results of the new method. The numerical procedure together with more complete numerical results will be published separately [28].

II. STANDARD MANY-BODY PERTURBATION THEORY

A. Time-independent perturbation theory

In the multi-reference form of MBPT we consider a number of *target states* that are eigenstates of the Hamiltonian of the system

$$H|\Psi^\alpha\rangle = E^\alpha|\Psi^\alpha\rangle \quad (\alpha = 1, 2, \dots, d). \quad (1)$$

The Hamiltonian is partitioned into a model Hamiltonian, H_0 , and a time-independent perturbation, H' ,

$$H = H_0 + H'. \quad (2)$$

For an N -electron system the model Hamiltonian is assumed to be composed of single-electron Schrödinger or Dirac Hamiltonians

$$H_0 = \sum_i^N h_0(i). \quad (3)$$

For each target state there is a model state, confined to a subspace, the *model space*, with the projection operator P . In the intermediate normalization we use here the model states are the projection of the corresponding target states on the model space

$$|\Psi_0^\alpha\rangle = P|\Psi^\alpha\rangle. \quad (4)$$

A wave operator can be defined for the inverse transformation

$$|\Psi^\alpha\rangle = \Omega|\Psi_0^\alpha\rangle \quad (\alpha = 1, 2, \dots, d). \quad (5)$$

An *effective Hamiltonian* can be defined, $H_{\text{eff}} = PH\Omega P$, that operates in the model space and for which the eigenvectors are the model states and the eigenvalues the corresponding exact energies

$$H_{\text{eff}}|\Psi_0^\alpha\rangle = E^\alpha|\Psi_0^\alpha\rangle. \quad (6)$$

The corresponding *effective interaction* is defined

$$V_{\text{eff}} = H_{\text{eff}} - PH_0P = PH'\Omega P. \quad (7)$$

The wave operator satisfies the generalized Bloch equation [29–31]

$$[\Omega, H_0]P = (H'\Omega - \Omega V_{\text{eff}})P. \quad (8)$$

This leads to the Rayleigh-Schrödinger perturbative expansion for a general multi-reference (quasidegenerate) model space, and it can also be used to generate the corresponding

linked-diagram expansion of Brueckner-Goldstone type

$$[\Omega, H_0]P = (H' \Omega - \Omega V_{\text{eff}})_{\text{linked}} P. \quad (9)$$

Here, only so-called linked terms or diagrams survive on the right-hand side. Using the exponential Ansatz

$$\Omega = \{e^S\}, \quad (10)$$

where the curly brackets represent normal-ordering, leads to the coupled-cluster expansion for the same model space [32]

$$[S, H_0]P = (H' \Omega - \Omega V_{\text{eff}})_{\text{conn}} P. \quad (11)$$

Here, all terms on the right-hand side are ‘‘connected.’’ (For the distinction between ‘‘linked’’ and ‘‘connected,’’ see, for instance, Ref. [1]).

B. Time-dependent perturbation theory

In this paper we shall only be concerned with *stationary states*, but we need for our purpose to use the formalism for time-dependent perturbation, which we shall briefly review.

The time-dependent state vector satisfies the time-dependent Schrödinger equation (using relativistic units $\hbar = c = m = \epsilon_0 = 1$)

$$i \frac{\partial}{\partial t} |\chi(t)\rangle = H(t) |\chi(t)\rangle, \quad (12)$$

where

$$H(t) = H_0 + H'(t). \quad (13)$$

H_0 is the time-independent model Hamiltonian and $H'(t)$ is a perturbation that might be time-dependent. In the *interaction picture* (IP), where an operator is related to that in the *Schrödinger picture* (SP) by

$$O_I(t) = e^{iH_0 t} O_S e^{-iH_0 t} \quad (14)$$

the Schrödinger equation becomes

$$i \frac{\partial}{\partial t} |\chi_I(t)\rangle = H'_I(t) |\chi_I(t)\rangle. \quad (15)$$

The *time-evolution operator* is defined by

$$|\chi_I(t)\rangle = U_I(t, t_0) |\chi_I(t_0)\rangle \quad (16)$$

and satisfies the equation

$$i \frac{\partial}{\partial t} U_I(t, t_0) = H'_I(t) U_I(t, t_0) \quad (17)$$

with the solution [33]

$$U_I(t, t_0) = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^t d^4 x_n \cdots \int_{t_0}^t d^4 x_1 \\ \times T_D[\mathcal{H}'_I(x_n) \mathcal{H}'_I(x_{n-1}) \cdots \mathcal{H}'_I(x_1)]. \quad (18)$$

Here, T_D is the Dyson time-ordering operator, and $\mathcal{H}'_I(x)$ is the perturbation *density*, defined by

$$H'_I(t) = \int d^3 x \mathcal{H}'_I(t, \mathbf{x}). \quad (19)$$

An *adiabatic damping* is added to the perturbation

$$H'_I(t) \rightarrow H'_{I\gamma} = H'_I e^{-\gamma|t|}; \quad U_I(t, t_0) \rightarrow U_{\gamma}(t, t_0), \quad (20)$$

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

C. Gell-Mann-Low theorem

A crucial component of our theoretical model is the *Gell-Mann-Low (GML) theorem*, which in its original form was presented already in 1951 [34]. According to this theorem, the wave function at time $t=0$ is for a single-reference model space given by

$$|\Psi\rangle = |\chi(0)\rangle = \lim_{\gamma \rightarrow 0} \frac{U_{\gamma}(0, -\infty) |\Psi_0\rangle}{\langle \Psi_0 | U_{\gamma}(0, -\infty) | \Psi_0 \rangle}, \quad (21)$$

where $|\Psi_0\rangle$ is the time-independent model state. It is assumed here that the perturbation H' is time-independent in the Schrödinger picture—apart from the adiabatic-damping factor. The wave function (21) satisfies a Schrödinger-type equation

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

The evolution operator normally contains singularities or quasi-singularities as $\gamma \rightarrow 0$, when an intermediate state is degenerate or closely degenerate with the initial state. In the GML formulas these (quasi)singularities are eliminated by the denominator so that the ratio is always regular, which is one formulation of the linked-diagram theorem [35].

We have in our previous work generalized this important theorem to the case of a general multi-reference model space [[4], Eq. (110)]

$$|\Psi^{\alpha}\rangle = \lim_{\gamma \rightarrow 0} \frac{N^{\alpha} U_{\gamma}(0, -\infty) |\Phi^{\alpha}\rangle}{\langle \Phi^{\alpha} | U_{\gamma}(0, -\infty) | \Phi^{\alpha} \rangle} \quad (\alpha = 1, 2, \dots, d), \quad (22)$$

where N^{α} is a normalization factor. The zeroth-order vector $|\Phi^{\alpha}\rangle$ is here defined as

$$|\Phi^{\alpha}\rangle = \lim_{\gamma \rightarrow 0} \lim_{t \rightarrow -\infty} |\chi^{\alpha}(t)\rangle. \quad (23)$$

Kuo *et al.* [36] have generalized the Gell-Mann law to the case of a degenerate model space, and then have found that it is sufficient that the zeroth-order function has a nonzero overlap with the target function. In the quasidegenerate case we have found that this is insufficient, and that the starting function for the theorem must be the limiting function above, which is an eigenfunction of the model Hamiltonian H_0 . This means that this function is generally distinct from the zeroth-order model function (4) (for further details, see our review paper [[4], Sec. 3.3]).

According to the generalized Gell-Mann-Low theorem the wave function (22) satisfies the time-independent Schrödinger-type equation

$$(H_0 + H')\Psi^{\alpha} = E^{\alpha}\Psi^{\alpha} \quad (\alpha = 1, 2, \dots, d), \quad (24)$$

where H' is, as before, the time-independent perturbation in the Schrödinger picture. This relation gives the important connection between energy-dependent MBPT and the stan-

standard energy-independent procedure and, therefore, forms the basis for the procedure developed here.

III. COVARIANT EVOLUTION-OPERATOR APPROACH

(The reader is referred to Refs. [4,5] for more details concerning the basic covariant evolution-operator formalism.)

A. Interaction with the electro-magnetic field

We consider now the interaction between electrons and the quantized electro-magnetic field represented by the perturbation density [37]

$$\mathcal{H}'_1(x) = -e\hat{\psi}_1^\dagger \alpha^\mu A_\mu \hat{\psi}_1. \quad (25)$$

Here, $\hat{\psi}_1, \hat{\psi}_1^\dagger$ are the electron field operators, α^μ the Dirac alpha operators and A_μ is the radiation field

$$A_\mu \propto \varepsilon_\mu^r [a_r^\dagger(\mathbf{k})e^{i\kappa x} + a_r(\mathbf{k})e^{-i\kappa x}], \quad (26)$$

applying standard summation convention. $a_r^\dagger(\mathbf{k}), a_r(\mathbf{k})$ are the photon creation/absorption operators, \mathbf{k} is the wave vector, κ is the four-vector momentum $\kappa = (\omega, -\mathbf{k})$ ($k = |\mathbf{k}|$), and ε_r^μ represent the polarization vectors. The Hamiltonian of the radiation field is represented by

$$H_{\text{rad}} = \omega a_r^\dagger(\mathbf{k})a_r(\mathbf{k}) = \mathbf{k}a_r^\dagger(\mathbf{k})a_r(\mathbf{k}). \quad (27)$$

With the interaction density (25) the evolution operator (18) for single-photon exchange becomes

$$U^{(2)}(t', t_0) = -\frac{1}{2} \int_{t_0}^{t'} \int_{t_0}^{t'} d^4x_1 d^4x_2 \hat{\psi}_{1+}^\dagger(x_1) \hat{\psi}_{1+}^\dagger(x_2) iI(x_1, x_2) \times \hat{\psi}_{1+}(x_2) \hat{\psi}_{1+}(x_1), \quad (28)$$

integrated over all space coordinates and time coordinates as indicated. $\hat{\psi}_{1+}, \hat{\psi}_{1+}^\dagger$ are the positive-energy part of the electron-field operators, and the interaction kernel

$$iI(x_1, x_2) = \overline{(-e\alpha^\mu A_\mu)_1 (-e\alpha^\nu A_\nu)_2} = e^2 \alpha_1^\mu \alpha_2^\nu iD_{F\mu\nu}(x_1 - x_2) \quad (29)$$

is given by the product of two perturbations (25) with contraction of the radiation-field operators (indicated by the hook). $D_{F\mu\nu}(x_1 - x_2)$ is the Feynman *photon propagator*.

The evolution operator above is *noncovariant* but can be made *covariant* by inserting zeroth-order two-particle Green's functions on the in- and outgoing states [3,4] [$G_0(x'_1, x'_2; x_1, x_2) = S_F(x'_1; x_1)S_F(x'_2; x_2)$, where $S_F(x'; x)$ represents the electron propagator or zeroth-order single-particle Green's function]

$$U_{\text{Cov}}^{(2)}(t', t_0) = -\frac{1}{2} \int \int d^3x'_1 d^3x'_2 \hat{\psi}_1^\dagger(x'_1) \hat{\psi}_1^\dagger(x'_2) \int \int d^4x_1 d^4x_2 \times G_0(x'_1, x'_2; x_1, x_2) \int \int d^3x_{10} d^3x_{20} iI(x_1, x_2) \times G_0(x_1, x_2; x_{10}, x_{20}) \hat{\psi}_1(x_{20}) \hat{\psi}_1(x_{10}), \quad (30)$$

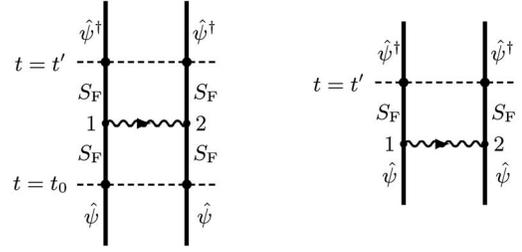


FIG. 1. Graphical representation of the covariant evolution operator for single-photon exchange in the form (30) (left) and in the form (31) with $t_0 \rightarrow -\infty$. The wavy lines represent covariant photons, and the free vertical lines represent single-electron Dirac states, generated in the nuclear potential. The lines between the heavy dots represent electron propagators (single-electron Green's functions).

as illustrated in Fig. 1 (left). Here, the time integrations over t_1 and t_2 are performed over *all times*, and positive- as well as negative-energy states are allowed as incoming and outgoing states. The initial and final times are the same for the two electrons, i.e.,

$$t_{10} = t_{20} = t_0 \quad \text{and} \quad t'_1 = t'_2 = t'.$$

We shall in the following assume that the initial time is $t_0 = -\infty$, and then due to the adiabatic damping (20) we can leave out the rightmost Green's function [4]

$$U_{\text{Cov}}^{(2)}(t', -\infty) = \frac{1}{2} \hat{\psi}_1^\dagger(x'_1) \hat{\psi}_1^\dagger(x'_2) G_0(x'_1, x'_2; x_1, x_2) \times iI(x_1, x_2) \hat{\psi}_1(x_2) \hat{\psi}_1(x_1) \quad (31)$$

(see Fig. 1 right). Here, we have left out the integrations, and in the following we shall also leave out the subscript Cov as well as the initial time.

B. Wave operator and effective interaction

The evolution operator is generally singular and can be expressed [4]

$$U(t)P = P + \tilde{U}(t)P \cdot PU(0)P, \quad (32)$$

where $\tilde{U}(t)$ is always regular and known as the *reduced evolution operator*—all singularities are collected in the last factor $PU(0)P$. The heavy dot indicates here that the two factors evolve in time independently from different model-space states (as further discussed in Sec. IV A). For the time $t=0$ this becomes

$$U(0)P = [1 + Q\tilde{U}(0)]P \cdot PU(0)P, \quad (33)$$

where Q is the projection operator for the “complementary space” (outside the model space).

Inserting the expression (33) into the GML formula (22), yields

$$\begin{aligned}
 |\Psi^\alpha\rangle &= [1 + Q\tilde{U}(0)]P \lim_{\gamma \rightarrow 0} \frac{N^\alpha U_\gamma(0, -\infty)|\Phi^\alpha\rangle}{\langle \Phi^\alpha | U_\gamma(0, -\infty) | \Phi^\alpha \rangle} \\
 &= [1 + Q\tilde{U}(0)]P |\Psi^\alpha\rangle.
 \end{aligned} \quad (34)$$

But $P|\Psi^\alpha\rangle = \Psi_0^\alpha$ is the model state (4), and hence the expression in the square brackets represents the wave operator (5),

$$\Omega = 1 + Q\tilde{U}(0). \quad (35)$$

The Q operator is for a two-electron system given by

$$Q = 1 - P = |rs\rangle\langle rs|, \quad (36)$$

where the ket vectors $|rs\rangle$ represent straight (nonantisymmetrized) products of single particle states, summed over all states outside the model space. The single-particle states are generated by the single-particle Hamiltonians (3)

$$h_0|i\rangle = \varepsilon_i|i\rangle, \quad (37)$$

which also include the nuclear field (Furry picture). In the two-electron system we shall study here, the occupied electron states are treated as open-shell or valence states, which implies that there are no core or hole states—apart from the negative-energy states.

Performing the integrations for the single-photon exchange (31), yields [3,4]

$$\begin{aligned}
 \langle rs|U^{(2)}(t)|ab\rangle &= \langle rs|e^{-it(E_{ab}-\varepsilon_r-\varepsilon_s)}\Gamma_Q(E_{ab})\mathcal{V}_1(E_{ab})|ab\rangle; \\
 E_{ab} &= \varepsilon_a + \varepsilon_b
 \end{aligned} \quad (38)$$

or, generally, operating on a model-space state of energy \mathcal{E} ,

$$U^{(2)}(t)P = e^{-it(\mathcal{E}-H_0)}\Gamma_Q(\mathcal{E})\mathcal{V}_1(\mathcal{E})P. \quad (39)$$

Here,

$$\Gamma_Q(\mathcal{E}) = \frac{Q}{\mathcal{E} - H_0} \quad (40)$$

is the *resolvent*, and

$$\begin{aligned}
 \langle rs|\mathcal{V}_1(\mathcal{E})|tu\rangle &= \langle rs| \int dk f(\mathbf{x}_1, \mathbf{x}_2, k) \\
 &\times \left[\frac{1}{\mathcal{E} - \varepsilon_r - \varepsilon_u - \text{sgn}(\varepsilon_r)(k - i\gamma)} \right. \\
 &\left. + \frac{1}{\mathcal{E} - \varepsilon_s - \varepsilon_t - \text{sgn}(\varepsilon_s)(k - i\gamma)} \right] |tu\rangle
 \end{aligned} \quad (41)$$

is the matrix element of the potential, considering both time orderings (see Fig. 2). Using the evolution operator (39) and the relation (35) (with $\tilde{U}^{(2)} = U^{(2)}$), this gives the wave operator for single-photon exchange

$$\Omega^{(1)}P = \Gamma_Q(\mathcal{E})\mathcal{V}_1(\mathcal{E})P. \quad (42)$$

The effective interaction (7) can generally be expressed [4]

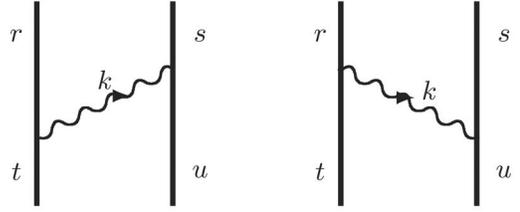


FIG. 2. Graphical representation of single-photon potential (41).

$$V_{\text{eff}} = P \left[i \frac{\partial}{\partial t} \tilde{U}(t) \right]_{t=0} P. \quad (43)$$

The reduced evolution operator has the same time dependence in all orders as in first-order (39), which implies that the time derivation eliminates the resolvent. In first-order this yields

$$V_{\text{eff}}^{(1)}(\mathcal{E}) = P\mathcal{V}_1(\mathcal{E})P. \quad (44)$$

The function $f(\mathbf{x}_1, \mathbf{x}_2, k)$ in the potential (41) depends on the gauge used and is in the Feynman gauge given by

$$f_{\text{F}}(\mathbf{x}_1, \mathbf{x}_2, k) = -\frac{e^2}{4\pi^2} (1 - \boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2) \frac{\sin(kr_{12})}{r_{12}},$$

where r_{12} is the interelectronic distance.

In the Coulomb gauge, which is natural to use in many-body calculations, the potential can be separated into an *instantaneous* and a *retarded* part,

$$V(\mathcal{E}) = V_{\text{I}} + V_{\text{Ret}}(\mathcal{E}), \quad (45)$$

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

$$V_{\text{I}} = V_{12} = \frac{e^2}{4\pi r_{12}}, \quad (46)$$

and the retarded part is given by the expression (41) with

$$\begin{aligned}
 f_{\text{C}}(\mathbf{x}_1, \mathbf{x}_2, k) &= -\frac{e^2}{4\pi^2} \left[-\boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2 \frac{\sin(kr_{12})}{r_{12}} + (\boldsymbol{\alpha}_1 \cdot \boldsymbol{\nabla}_1) \right. \\
 &\left. \times (\boldsymbol{\alpha}_2 \cdot \boldsymbol{\nabla}_2) \frac{\sin(kr_{12})}{k^2 r_{12}} \right],
 \end{aligned} \quad (47)$$

where the nabla operators do not operate beyond the square bracket. Here, the first term represent the *Gaunt* part and the second term the *scalar-retardation* part, which together form the *Breit interaction*. In the following we shall assume that the Coulomb gauge is used.

The relations given here, particularly the equations (35) and (43), demonstrate the close analogy between the covariant evolution-operator approach and standard MBPT, which opens up the possibility for a merger of the two procedures.

IV. DEVELOPMENT OF A MANY-BODY-QED PROCEDURE. BLOCH EQUATION FOR INSTANTANEOUS AND RETARDED INTERACTIONS

A. Retarded interactions

From the definition (32), the following relation can be derived, using standard algebra [5],

$$\tilde{U}(t)P = \bar{U}(t)P + \tilde{U}(t)P\bar{U}(0)P - \tilde{U}(t)P \cdot P\bar{U}(0). \quad (48a)$$

In the product $\tilde{U}(t)P\bar{U}(0)P$ the time-dependent part, $\tilde{U}(t)$, evolves from the energy of the state to the far right (\mathcal{E}) and, therefore, depends on this energy. In the dot product, $\tilde{U}(t) \cdot P\bar{U}(0)P$, on the other hand, the operator $\tilde{U}(t)$ evolves from the energy of the intermediate state (\mathcal{E}_1). More explicitly, we can then express the relation (48a) as

$$\tilde{U}(\mathcal{E}, t)P = \bar{U}(\mathcal{E}, t)P + \tilde{U}(\mathcal{E}, t)P_1\bar{U}(\mathcal{E}, 0)P - \tilde{U}(\mathcal{E}_1, t)P_1\bar{U}(\mathcal{E}, 0)P, \quad (48b)$$

where P (P_1) represents a model-space state of energy \mathcal{E} (\mathcal{E}_1). ‘‘Ubar’’ represents the evolution operator without intermediate model-space states,

$$\bar{U}(t)P = \tilde{U}(t)P - M(t), \quad (49)$$

and M is the *model-space contribution* (MSC). From the relation above we then find that the latter part becomes

$$M = [\tilde{U}(\mathcal{E}, t) - \tilde{U}(\mathcal{E}_1, t)]P_1\bar{U}(\mathcal{E}, 0)P. \quad (50)$$

U and \tilde{U} have the general form in analogy with the first-order result (39), i.e., a resolvent with an energy denominator (in this case equal to $\mathcal{E} - \mathcal{E}_1$) and a corresponding time exponential. Introducing the effective interaction without MSC, \bar{V}_{eff} , in analogue with the interaction (43),

$$\bar{V}_{\text{eff}} = P \left[i \frac{\partial}{\partial t} \bar{U}(t) \right]_{t=0} P, \quad (51)$$

we find as before that the time derivative eliminates the energy denominator. We then have

$$P_1\bar{U}(\mathcal{E}, 0)P = \frac{\bar{V}_{\text{eff}}(\mathcal{E})}{\mathcal{E} - \mathcal{E}_1},$$

and

$$M = \frac{\tilde{U}(\mathcal{E}) - \tilde{U}(\mathcal{E}_1)}{\mathcal{E} - \mathcal{E}_1} \bar{V}_{\text{eff}} = \frac{\delta \tilde{U}}{\delta \mathcal{E}} \bar{V}_{\text{eff}}, \quad (52)$$

using the difference ratio defined in Appendix B. This gives with the relation (49)

$$\tilde{U}(t)P = \bar{U}(t)P + \frac{\delta \bar{U}}{\delta \mathcal{E}} \bar{V}_{\text{eff}}. \quad (53)$$

With the wave-operator relation (35) we then have

$$\Omega P = \bar{\Omega} P + \frac{\delta \bar{\Omega}}{\delta \mathcal{E}} \bar{V}_{\text{eff}}, \quad (54)$$

where the last term represents the MSC (including ‘‘folded’’ diagram) and $\bar{\Omega}$ is the wave operator without MSC.

The relation (48a) leads to the expansion

$$\begin{aligned} \tilde{U}(t)P &= \bar{U}(t)P + \tilde{U}(t)(P\bar{U}P - \cdot P\bar{U}P) + \bar{U}(t)(P\bar{U}P - \cdot P\bar{U}P) \\ &\quad \times (P\bar{U}P - \cdot P\bar{U}P) + \dots \end{aligned} \quad (55)$$

The exchange of a single photon corresponds to the second-order evolution operator and leads to the result given above (42). The two-photon exchange corresponds to the next even order of the evolution operator

$$\tilde{U}^{(4)}(t)P = \bar{U}^{(4)}(t)P + \bar{U}^{(2)}(t)(P\bar{U}^{(2)}P - \cdot P\bar{U}^{(2)}P). \quad (56)$$

Since there is no MSC in lowest order, we have $U^{(2)} = \bar{U}^{(2)} = \tilde{U}^{(2)}$, and the corresponding wave operator becomes

$$\Omega^{(2)}P = Q\tilde{U}^{(4)}(0)P = \bar{\Omega}^{(2)}P + \frac{\delta \bar{\Omega}^{(1)}}{\delta \mathcal{E}} V_{\text{eff}}^{(1)}, \quad (57)$$

where $\bar{\Omega}^{(2)}P = \Gamma_Q \mathcal{V}_1 \Gamma_Q \mathcal{V}_1 P$. In the case of degeneracy this goes over into

$$\Omega^{(2)}P = \bar{\Omega}^{(2)}P + \frac{\partial \bar{\Omega}^{(1)}}{\partial \mathcal{E}} V_{\text{eff}}^{(1)}. \quad (58)$$

In third order we have [[5], Appendix D]

$$\Omega^{(3)}P = \bar{\Omega}^{(3)}P + \frac{\delta \bar{\Omega}^{(2)}}{\delta \mathcal{E}} V_{\text{eff}}^{(1)} + \frac{\delta \bar{\Omega}^{(1)}}{\delta \mathcal{E}} \bar{V}_{\text{eff}}^{(2)}, \quad (59)$$

which leads to

$$\Omega^{(3)}P = \bar{\Omega}^{(3)}P + \frac{\delta \bar{\Omega}^{(1)}}{\delta \mathcal{E}} V_{\text{eff}}^{(2)} + \frac{\delta \bar{\Omega}^{(2)}}{\delta \mathcal{E}} V_{\text{eff}}^{(1)} + \frac{\delta^2 \bar{\Omega}^{(1)}}{\delta \mathcal{E}^2} (V_{\text{eff}}^{(1)})^2, \quad (60)$$

where the second-order difference ratio is defined in Appendix B. The last term is associated with double model-space contributions (‘‘double fold’’). This leads to conjecture for the all-order expansion [cf. [5], Eq. (116)]

$$\Omega P = \bar{\Omega} P + \sum_{n=1}^{\infty} \frac{\delta^n \bar{\Omega}}{\delta \mathcal{E}^n} (V_{\text{eff}})^n, \quad (61)$$

which we shall now verify.

In order to prove the relation above, we start by using this relation to form the difference ratio

$$\begin{aligned} \frac{\delta \Omega}{\delta \mathcal{E}} &= \frac{\delta \bar{\Omega}}{\delta \mathcal{E}} + \frac{\delta^2 \bar{\Omega}}{\delta \mathcal{E}^2} V_{\text{eff}} + \frac{\delta^3 \bar{\Omega}}{\delta \mathcal{E}^3} (V_{\text{eff}})^2 + \dots \\ &\quad + \frac{\delta \bar{\Omega}}{\delta \mathcal{E}} \frac{\delta V_{\text{eff}}}{\delta \mathcal{E}} + \frac{\delta^2 \bar{\Omega}}{\delta \mathcal{E}^2} V_{\text{eff}} \frac{\delta V_{\text{eff}}}{\delta \mathcal{E}} + \dots \\ &= \sum_{n=1}^{\infty} \frac{\delta^n \bar{\Omega}}{\delta \mathcal{E}^n} (V_{\text{eff}})^{(n-1)} \left[1 + \frac{\delta V_{\text{eff}}}{\delta \mathcal{E}} \right]. \end{aligned} \quad (62)$$

[It should be noted that the different V_{eff} operators are in general associated with different energies, as explained in Appendix B, Eq. (B8).] Next, we take the time derivative of the relation (53), using the relation (43), which yields

$$V_{\text{eff}} = \left[1 + \frac{\delta V_{\text{eff}}}{\delta \mathcal{E}} \right] \bar{V}_{\text{eff}}. \quad (63)$$

This gives with the relation (62)

$$\frac{\delta \Omega}{\delta \mathcal{E}} \bar{V}_{\text{eff}} = \sum_{n=1}^{\infty} \frac{\delta^n \bar{\Omega}}{\delta \mathcal{E}^n} (V_{\text{eff}})^n, \quad (64)$$

and with the relation (53) we retrieve the relation (61), which is then proven.

In order to obtain more Bloch-type relations, we first introduce the *reaction operator*, which is the effective interaction (43), apart from the projection operators,

$$V_{\text{R}} = \left[i \frac{\partial}{\partial t} \bar{U}(t) \right]_{t=0}. \quad (65)$$

This gives $V_{\text{eff}} = P V_{\text{R}} P$, and the reaction operator is equal to the wave operator, apart from the resolvent,

$$Q \bar{U}(0) = Q \Omega = \Gamma_Q V_{\text{R}}. \quad (66)$$

We also introduce the operator

$$\bar{V}_{\text{R}} = \left[i \frac{\partial}{\partial t} \bar{U}(t) \right]_{t=0}, \quad (67)$$

where \bar{U} is the evolution operator without MSC. This leads in analogy with the relation (66) to

$$Q \bar{U}(0) = Q \bar{\Omega} = \Gamma_Q \bar{V}_{\text{R}}. \quad (68)$$

Using the rule for differentiating a product, developed in Appendix B [Eq. (B4)], and the relation

$$\begin{aligned} \frac{\delta^n \Gamma_Q(\mathcal{E})}{\delta \mathcal{E}^m} &= (-1)^m \Gamma_Q(\mathcal{E}) \Gamma_Q(\mathcal{E}_1) \cdots \Gamma_Q(\mathcal{E}_m) \\ &= -\Gamma_Q(\mathcal{E}) \frac{\delta^{(m-1)} \Gamma_Q(\mathcal{E}_1)}{\delta \mathcal{E}_1^{(m-1)}}, \end{aligned} \quad (69)$$

we can express the difference ratios of $\bar{\Omega}$ as

$$\begin{aligned} \frac{\delta^n \bar{\Omega}(\mathcal{E})}{\delta \mathcal{E}^n} &= \frac{\delta^n}{\delta \mathcal{E}^n} [\Gamma_Q(\mathcal{E}) \bar{V}_{\text{R}}(\mathcal{E})] \\ &= \sum_{m=0}^n \frac{\delta^n \Gamma_Q(\mathcal{E})}{\delta \mathcal{E}^m} \frac{\delta^{(n-m)} \bar{V}_{\text{R}}(\mathcal{E}_m)}{\delta \mathcal{E}_m^{(n-m)}} \\ &= \Gamma_Q(\mathcal{E}) \frac{\delta^n \bar{V}_{\text{R}}(\mathcal{E})}{\delta \mathcal{E}^n} \\ &\quad - \sum_{m=1}^n \Gamma_Q(\mathcal{E}) \frac{\delta^{(m-1)} \Gamma_Q(\mathcal{E}_1)}{\delta \mathcal{E}_1^{(m-1)}} \frac{\delta^{(n-m)} \bar{V}_{\text{R}}(\mathcal{E}_m)}{\delta \mathcal{E}_m^{(n-m)}}. \end{aligned} \quad (70)$$

The last term can be expressed

$$-\Gamma_Q(\mathcal{E}) \sum_{m=0}^{n-1} \frac{\delta^n \Gamma_Q(\mathcal{E}_1)}{\delta \mathcal{E}^m} \frac{\delta^{(n-m-1)} \bar{V}_{\text{R}}(\mathcal{E}_m)}{\delta \mathcal{E}_m^{(n-m-1)}} = -\Gamma_Q(\mathcal{E}) \frac{\delta^{(n-1)} \bar{\Omega}(\mathcal{E}_1)}{\delta \mathcal{E}_1^{(n-1)}}. \quad (71)$$

Inserted in the expansion (61), the last term yields

$$-\sum_{n=1}^{\infty} \Gamma_Q(\mathcal{E}) \left[\frac{\delta^{(n-1)} \bar{\Omega}(\mathcal{E}_1)}{\delta \mathcal{E}_1^{(n-1)}} (V_{\text{eff}})^{(n-1)} \right] V_{\text{eff}} = -\Gamma_Q \Omega V_{\text{eff}} \quad (72)$$

Finally, we have the relation

$$Q \Omega P = Q \bar{\Omega} P - \Gamma_Q \Omega V_{\text{eff}} + \Gamma_Q \sum_{n=1}^{\infty} \frac{\delta^n \bar{V}_{\text{R}}}{\delta \mathcal{E}^n} (V_{\text{eff}})^n, \quad (73)$$

which will later be used to derive the Bloch equations for energy-dependent interactions.

B. Instantaneous interactions

The instantaneous Coulomb interaction can be treated essentially as in standard (relativistic) many-body theory, and we start by recalling the treatment of the correlation effect for a two-electron system. The wave operator in the coupled-cluster formalism (10) can then be expressed [1]

$$\Omega = 1 + S_2, \quad (74)$$

where S_2 is the two-body cluster operator. Operating on a model-space state, yields a *pair function*

$$|\rho_{ab}\rangle = \Omega |ab\rangle = |ab\rangle + s_{ab}^{rs} |rs\rangle. \quad (75)$$

Inserting the pair function into the Bloch equation (11), yields the corresponding pair equation

$$\begin{aligned} &[\varepsilon_a + \varepsilon_b - h_0(1) - h_0(2)] |\rho_{ab}\rangle \\ &= |rs\rangle \langle rs | V_{12} | \rho_{ab} \rangle - |\rho_{cd}\rangle \langle cd | V_{\text{eff}} | ab \rangle. \end{aligned} \quad (76)$$

The last term is the *folded* term and is the result of the reduction of singularities which appear when the intermediate states lie in the model space, which we have referred to above as *model-space contribution* (MSC). When the equation is solved iteratively, the Coulomb interactions are generated to all orders, as illustrated in Fig. 3. This is the type of pair functions we have been using in our many-body calculations for several decades [38–42].

We denote the wave operator with only Coulomb interactions by Ω_1 and the part with no folded diagrams by $\bar{\Omega}_1$. Then we have

$$\bar{\Omega}_1 P = [1 + \Gamma_Q V_{12} + \Gamma_Q V_{12} \Gamma_Q V_{12} + \cdots] P, \quad (77)$$

and using the relations (73) and (61), this leads to the standard Bloch equation (8)

$$[\Omega_1, H_0] P = V_{12} \Omega_1 P - \Omega_1 V_{\text{eff}}. \quad (78)$$

C. Combined instantaneous and retarded interactions

We shall now find Bloch equations for the *combined* retarded and instantaneous interactions. In the Coulomb gauge

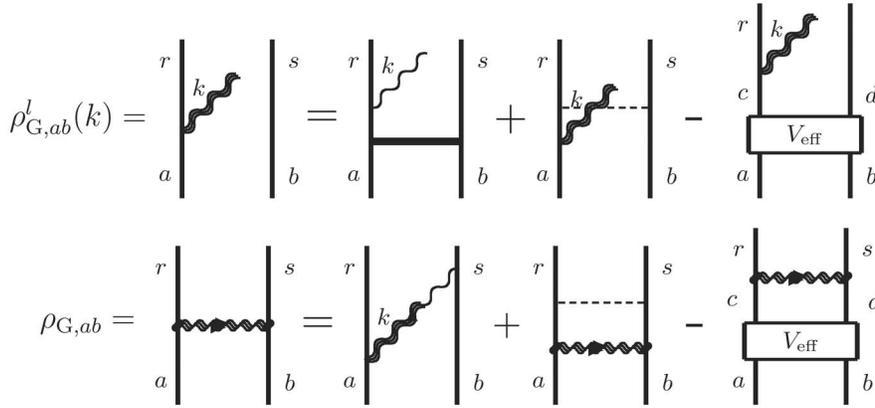


FIG. 4. Graphical representation the pair equations (92), solving the Bloch equations [Eqs. (89) and (91)].

$$Q\Omega_G^l(k)P = \Gamma_Q V_G^l(k)\Omega_l P + \Gamma_Q V_{12}\Omega_G^l(k)P - \Gamma_Q \Omega_G^l(k)V_{\text{eff}} \quad (88)$$

and to the Bloch equation

$$[\Omega_G^l(k), H_0]P = V_G^l(k)\Omega_l P + V_{12}\Omega_G^l(k)P - \Omega_G^l(k)V_{\text{eff}}. \quad (89)$$

In the next step the photon of the function $\Omega_G^l(k)$ is being absorbed by the other electron, followed by additional Coulomb iterations. We denote the corresponding wave operator by Ω_G . Omitting for the time being the MSC associated with the Coulomb interactions, this leads to

$$\bar{\Omega}_G P = (1 + \Gamma_Q V_{12} + \Gamma_Q V_{12}\Gamma_Q V_{12} + \dots)\Gamma_Q V_G^l(k)\Omega_G^l(k)P, \quad (90)$$

integrating over k and summing over l according to the relation (79). The MSC are as before obtained by inserting this relation into the formula (73), which—using the same argument as before—yields

$$[\Omega_G, H_0]P = V_G^l(k)\Omega_G^l(k)P + V_{12}\Omega_G P - \Omega_G V_{\text{eff}}. \quad (91)$$

The equations above represent our main equations for dealing with the combined retarded and unretarded interactions. For a two-electron system they can be converted to the pair equations

$$\begin{aligned} & [\varepsilon_a + \varepsilon_b - h_0(1) - h_0(2) - k]|\rho_{G,ab}^l(k)\rangle \\ & = |rs\rangle\langle rs|V_G^l(k)|\rho_{ab}\rangle + |rs\rangle\langle rs|V_{12}|\rho_{G,ab}^l(k)\rangle \\ & \quad - |\rho_{G,cd}^l(k)\rangle\langle cd|V_{\text{eff}}|ab\rangle \\ & [\varepsilon_a + \varepsilon_b - h_0(1) - h_0(2)]|\rho_{G,ab}\rangle \\ & = |rs\rangle\langle rs|V_G^l(k)|\rho_{ab}^l(k)\rangle + |rs\rangle\langle rs|V_{12}|\rho_{G,ab}\rangle \\ & \quad - |\rho_{G,cd}\rangle\langle cd|V_{\text{eff}}|ab\rangle. \end{aligned} \quad (92)$$

Note that the first of these equations is deduced from the relation (89) with the extended H_0 , which leads to the momentum k on the left-hand side. These equations, which can be solved using standard technique [43,44], are illustrated in Fig. 4. In Figs. 5 and 6 (upper line) we show more explicitly the diagrams involved in the process just described—in the former case without any Coulomb interactions before and after the retarded interaction and in the latter case with such interactions.

When the photon is instead absorbed by the same electron as it is emitted from, we get the corresponding self-energy and vertex-correction effects—of course, after appropriate renormalization—as indicated in the bottom lines of the same figures.

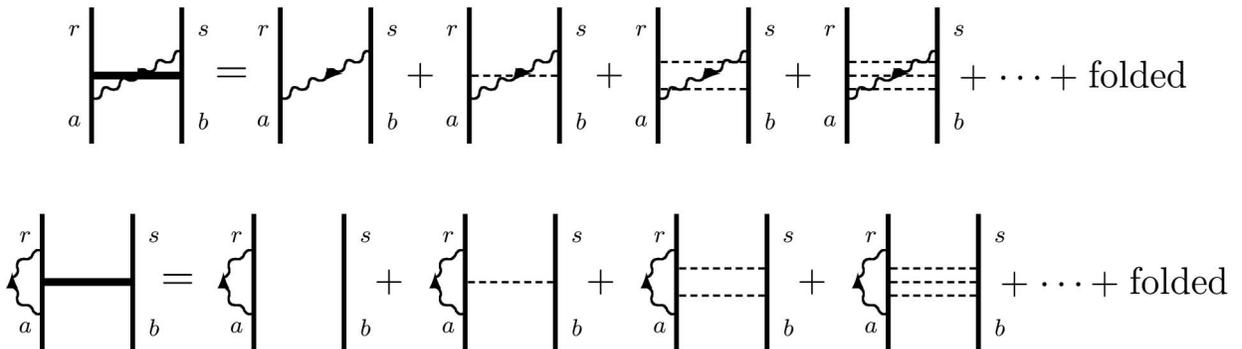


FIG. 5. Graphical representation of a single retarded photon with crossing Coulomb interactions and without Coulomb interactions before and after the retarded interaction.

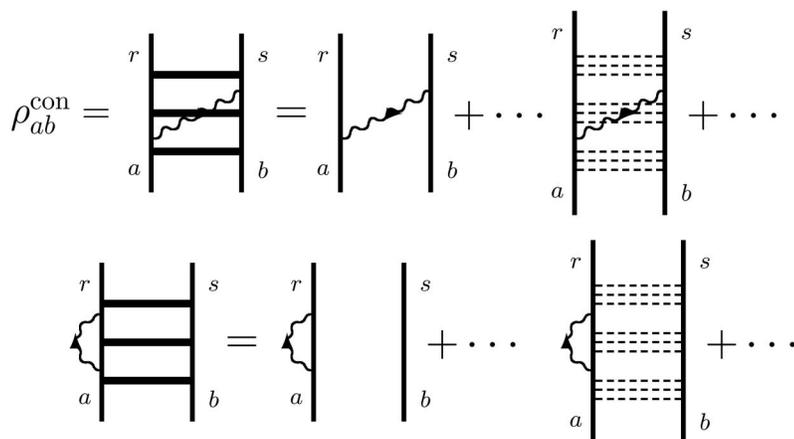


FIG. 6. Graphical representation of a single retarded photon with crossing Coulomb interactions and with Coulomb interactions before and after the retarded interaction. The diagrams in upper line are obtained by solving the pair equations (92) and those in lower line by analogous equation.

D. Derivation of the general Bloch equations

The Bloch equations derived above are valid only in the case of no more than one uncontracted photon at each instance. In order to derive the more general *Fock-space Bloch equation*, we can proceed exactly as in the energy-independent case [29], starting from the Schrödinger-type equation (80). We first project this equation on the model space

$$P(H_0 + H')\Omega\Psi_0^\alpha = H_0\Psi_0^\alpha + PH'\Omega\Psi_0^\alpha = E^\alpha\Psi_0^\alpha, \quad (93)$$

using the fact that P and H_0 commute, and then operate from the left with Ω

$$\Omega H_0\Psi_0^\alpha + \Omega PH'\Omega\Psi_0^\alpha = E^\alpha\Psi_0^\alpha. \quad (94)$$

Subtracting the original SE (24), then yields the *Fock-space Bloch equation*

$$[\Omega, H_0]P = H'\Omega P - \Omega V_{\text{eff}}, \quad H_{\text{eff}} = PH_0P + V_{\text{eff}},$$

$$V_{\text{eff}} = PH'\Omega P, \quad (95)$$

The solution can be expressed

$$\Omega P = \Gamma_Q(H'\Omega - \Omega V_{\text{eff}})P, \quad (96)$$

where Γ_Q is the generalized resolvent (82).

We can expand the Fock-space wave operator and resolvent into components acting in the subspace with no photons, with one photon, etc. as

$$\begin{aligned} \Omega &= \Omega + \Omega^+ + \dots, \\ \Gamma_Q &= \Gamma_Q + \Gamma_Q^+ \dots \end{aligned} \quad (97)$$

The generalized Bloch equation (96) can then be separated into

$$\begin{aligned} \Omega P &= P + \Gamma_Q[V_{12}\Omega + \overline{V_{\text{Ret}}}\Omega^+ - \Omega V_{\text{eff}}]P \\ \Omega^+ P &= \Gamma_Q^+[V_{\text{Ret}}\Omega + V_{12}\Omega^+ + \overline{V_{\text{Ret}}}\Omega^{++} - \Omega^+ V_{\text{eff}}]P \\ \Omega^{++} P &= \dots \end{aligned} \quad (98)$$

The hook represents integration over the photon momentum k and summation over the angular momentum l , according to

the single-photon expression (79). These equations are valid also in the case of multiple free photons at the same time and can, therefore, be used for the evaluation of irreducible diagrams with several retarded photons (see Fig. 8). Considering at most a single free photon, we see that they lead to the Bloch equations (89) and (91) derived above.

V. NUMERICAL PROCEDURE AND RESULTS

The pair equations (92) considered here can be solved numerically with essentially the same technique as developed by Salomonson and Öster for (relativistic) many-body calculations [43,44] and used in our previous works [3,45]. The radial integrations are performed with an exponential grid with 70–150 grid points and the k integration with 100–150 points using Gaussian quadrature. For excited states, poles appear in the k integration, which require special attention (for details, see Ref. [45]). The numerical calculations are quite time consuming in the present case, since separate pair functions have to be constructed for each value of the photon momentum. On the other hand, the procedure is particularly well suited for parallel computing, and we hope that the procedure can be speeded up considerably, when our routines are better optimized.

Here, we shall only give some illustrative examples of our numerical results—more results will be published separately [28]. In Table I we show the effect of one retarded photon

TABLE I. Effects of one- and two-photon exchange on the energy of the excited $1s2s^1S$ and 3S states of heliumlike neon (in μH).

		$1s2s^1S$	$1s2s^3S$
One-photon	Gaunt	2465.44	171.50
	Scalar ret.	171.58	-171.58
Two-photon (noncrossing)	Coul.-Gaunt	-794.8	-51.8
	Coul.-Scal.ret.	22.5	42.5
One + two-photon	Gaunt	1670.7	119.7
	Scal.ret.	194.2	-129.1
One photon correlated	Gaunt	1752.0	124.6
	Scal.ret.	183.9	-132.2

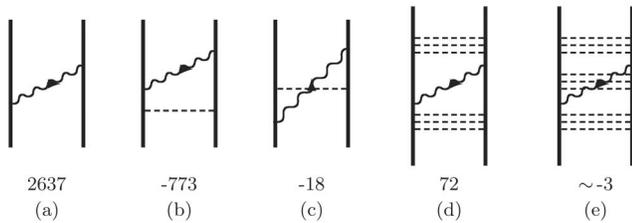


FIG. 7. Diagrams evaluated for the $1s2s^1S$ and $1s2s^3S$ states of heliumlike neon with the results given in Table I. [The numbers represent the energy contributions to the singlet state in μH . The result (c) is taken from our previous work [45] and (e) is so far only estimated.]

with one and infinitely many noncrossing Coulomb interactions for the $1s2s^1S$ and 3S states of heliumlike neon, excluding virtual pairs (NVP). This corresponds to the diagrams shown in Fig. 7. Figures 7(c) and 7(e) have not yet been evaluated in the present work but calculations are underway. Fig. 7(c) was previously evaluated by means of S -matrix method [45], and the result of Fig. 7(e) is presently estimated.

The two-photon effect [Fig. 7(b)] has been compared with the corresponding S -matrix results [45] and are found to agree to 3-4 digits, which represents the numerical accuracy of the present calculations. The effect of correlation beyond the second-order [Figs. 7(d) and 7(e)] is in this case found to be about ten percent of the two-photon effect [Fig. 7(b)] and in turn one order of magnitude larger than the effect of the retarded two-photon interaction [45] in Fig. 8. The effect of virtual pairs is of the same order as that of two retarded interactions. This indicates that for heliumlike neon the procedure described here with a single retarded photon together with Coulomb interactions is capable of reproducing about 99% of the nonradiative effects not included in a standard many-body perturbation treatment with only instantaneous Coulomb interactions. By including the effect of two retarded photons that can be evaluated by standard method, the energy contributions beyond standard relativistic MBPT can for heliumlike neon be reproduced to something like 99.8%–99.9%.

VI. SUMMARY AND OUTLOOK

We have, in previous articles, described a new technique for QED calculations that we refer to as the covariant

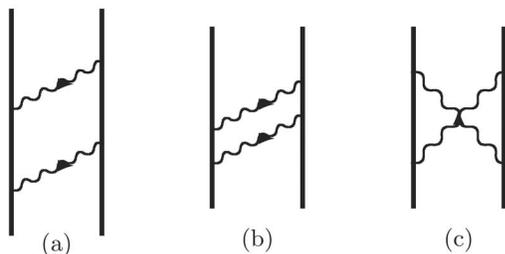


FIG. 8. Reducible (a) and irreducible (b) and (c) two-photon diagrams that have previously been evaluated [45].

evolution-operator (CEO) method [2–5]. This method has the great advantage compared to other QED techniques that it has a structure very akin to that of standard many-body perturbation theory, which opens up the possibility for a merger of the two techniques. In two previous papers [4,5] we have indicated how such a merger can be accomplished, and this is developed further in the present paper into a rigorous many-body-QED procedure. Some preliminary numerical results are presented. Combined QED and correlation effects, which can be treated only in a very limited fashion by standard techniques, are of particular importance for light and medium-heavy elements. The CEO method also has the advantage compared to the standard S -matrix technique that it can be applied to the case of quasidegeneracy (a property it shares with the two-times Green's-function technique of Shaev *et al.* [14]).

The numerical procedure we have developed so far represents the exchange of a single retarded photon and an arbitrary number of instantaneous Coulomb interactions between the electrons, crossing and noncrossing. We have been working with positive-energy intermediate states—no-virtual-pair (NVP) approximation—but single and double virtual pairs can be included in the procedure. The procedure can also be used—with proper renormalization—for radiative effects (self-energy and vertex corrections) with a single retarded photon (see Figs. 6 and 5). In principle, the procedure can be used also for *irreducible* multi-photon effects, where retarded interactions overlap in time, like those indicated in Figs. 8(b) and 8(c), by treating more than one uncontracted photon at a particular time. At present, however, this is beyond reach with the computers we have available. On the other hand, *reducible* multi-photon effects, where the interactions are separated in time, as illustrated in Fig. 8(a), can already be included at present by repeated use of the procedure described.

It has been demonstrated that one retarded photon with Coulomb interaction represents by far the dominating part of the nonradiative multi-photon exchange for light and medium-heavy elements beyond the standard Coulomb correlation (of the order of 99% for heliumlike neon), and the situation can be expected to be similar for the radiative part. The small effects due to two irreducible retarded photons without Coulomb interactions can be evaluated with standard QED methods, and combining the two methods would yield something like 99.8%–99.9% of the effects beyond standard MBPT. Higher-order effects can with good accuracy be estimated by means of analytical approximations. Therefore, it is our belief that the method presented here, when the routines are fully developed, should be able to produce accurate results for energy separations, such as the fine-structure separations, for light and medium-heavy elements, hopefully down to neutral helium.

ACKNOWLEDGMENTS

The authors wish to express their thanks to Björn Åsén for valuable discussions. The work has been supported by the Swedish Research Council.

APPENDIX A: COULOMB-GAUGE INTERACTION

The terms in the Coulomb-gauge expression (47) can be separated into a product of two single-particle potentials by the spherical wave expansion, using the relation

$$\frac{\sin(kr_{12})}{r_{12}} = k \sum_{l=0}^{\infty} (2l+1) j_l(kr_1) j_l(kr_2) \mathbf{C}^l(1) \cdot \mathbf{C}^l(2), \quad (\text{A1})$$

where \mathbf{C}^l is a spherical tensor, associated with the spherical harmonics Y^l . The Gaunt term then becomes

$$\sum_{l=0}^{\infty} V_G^l(kr_1) \cdot V_G^l(kr_2), \quad (\text{A2})$$

where $V_G^l(kr_i)$ is

$$V_G^l(kr) = \frac{e}{2\pi} \sqrt{k(2l+1)} \boldsymbol{\alpha} j_l(kr) \mathbf{C}^l. \quad (\text{A3})$$

For the scalar-retardation term we use the relation ([46], Sec. 5.7) ([47], Part II, Appendix A)

$$\begin{aligned} \nabla[f(r) \mathbf{C}_m^l] = & \frac{1}{2l+1} \left[-\sqrt{(l+1)(2l+3)} \left(\frac{d}{dr} - \frac{l}{r} \right) f(r) \mathbf{C}_m^{l,l+1} \right. \\ & \left. + \sqrt{l(2l-1)} \left(\frac{d}{dr} + \frac{l+1}{r} \right) f(r) \mathbf{C}_m^{l,l-1} \right], \quad (\text{A4}) \end{aligned}$$

where $\mathbf{C}_m^{l,l\pm 1}$ is a vector, associated with the vector spherical harmonics $\mathbf{Y}_m^{l,l\pm 1}$, and the relation

$$\boldsymbol{\alpha} \cdot \mathbf{C}_m^{l,k} = \{\boldsymbol{\alpha} \mathbf{C}_m^l\}_k, \quad (\text{A5})$$

where the left-hand side is a scalar product and the right-hand side a tensor product. Together with [48]

$$\left(\frac{d}{dr} - \frac{l}{r} \right) j_l(kr) = -kj_{l+1}(kr), \quad (\text{A6})$$

$$\left(\frac{d}{dr} + \frac{l+1}{r} \right) j_l(kr) = kj_{l-1}(kr), \quad (\text{A7})$$

the final result of the scalar retardation term becomes

$$- \sum_{l=0}^{\infty} V_{\text{SR}}^l(kr_1) V_{\text{SR}}^l(kr_2), \quad (\text{A8})$$

where expression for the single-particle potentials for the scalar retardation is written as

$$\begin{aligned} V_{\text{SR}}^l(kr) = & \frac{e}{2\pi} \sqrt{\frac{k}{2l+1}} \left[\sqrt{(l+1)(2l+3)} j_{l+1}(kr) \{\boldsymbol{\alpha} \mathbf{C}^{l+1}\}^l \right. \\ & \left. + \sqrt{l(2l-1)} j_{l-1}(kr) \{\boldsymbol{\alpha} \mathbf{C}^{l-1}\}^l \right]. \quad (\text{A9}) \end{aligned}$$

The function, $f(k)$, in the Coulomb gauge expression (47) then becomes

$$f(k) = \sum_{l=0}^{\infty} [V_G^l(kr_1) V_G^l(kr_2) - V_{\text{SR}}^l(kr_1) V_{\text{SR}}^l(kr_2)]. \quad (\text{A10})$$

APPENDIX B: RULES FOR DIFFERENTIATION

The difference ratios we use in the formalism presented here are of a special kind and give rise to special handling rules (see also Ref. [5], Appendix E).

If $A(\mathcal{E})$ is an operator function of the (energy) parameter \mathcal{E} , then we define the first-order difference ratio

$$\frac{\delta A(\mathcal{E})}{\delta \mathcal{E}} = \frac{\delta_{\mathcal{E}\mathcal{E}_1} A(\mathcal{E})}{\delta \mathcal{E}} = \frac{A(\mathcal{E}) - A(\mathcal{E}_1)}{\mathcal{E} - \mathcal{E}_1}.$$

Then

$$\frac{\delta}{\delta \mathcal{E}} [A(\mathcal{E}) B(\mathcal{E})] = \frac{\delta_{\mathcal{E}\mathcal{E}_1} A(\mathcal{E})}{\delta \mathcal{E}} B(\mathcal{E}_1) + A(\mathcal{E}) \frac{\delta_{\mathcal{E}\mathcal{E}_1} B(\mathcal{E})}{\delta \mathcal{E}}. \quad (\text{B1})$$

The second difference ratio is defined as

$$\frac{\delta^2 A(\mathcal{E})}{\delta \mathcal{E}^2} = \frac{\delta_{\mathcal{E}\mathcal{E}_1\mathcal{E}_2}^2 A(\mathcal{E})}{\delta \mathcal{E}^2} = \frac{\delta_{\mathcal{E}\mathcal{E}_1}}{\delta \mathcal{E}} \frac{\delta_{\mathcal{E}\mathcal{E}_2}}{\delta \mathcal{E}} A(\mathcal{E})$$

and generally

$$\frac{\delta_{\mathcal{E}\mathcal{E}_1 \dots \mathcal{E}_n}^n}{\delta \mathcal{E}^n} = \frac{\delta_{\mathcal{E}\mathcal{E}_1}}{\delta \mathcal{E}} \frac{\delta_{\mathcal{E}\mathcal{E}_2}}{\delta \mathcal{E}} \dots \frac{\delta_{\mathcal{E}\mathcal{E}_n}}{\delta \mathcal{E}}.$$

It then follows that

$$\begin{aligned} \frac{\delta^2}{\delta \mathcal{E}^2} [A(\mathcal{E}) B(\mathcal{E})] &= \frac{\delta_{\mathcal{E}\mathcal{E}_1\mathcal{E}_2}^2}{\delta \mathcal{E}^2} [A(\mathcal{E}) B(\mathcal{E})] \\ &= \frac{\delta_{\mathcal{E}\mathcal{E}_1}}{\delta \mathcal{E}} \frac{\delta_{\mathcal{E}\mathcal{E}_2}}{\delta \mathcal{E}} [A(\mathcal{E}) B(\mathcal{E})] \\ &= \frac{\delta_{\mathcal{E}\mathcal{E}_1}}{\delta \mathcal{E}} \left[\frac{\delta_{\mathcal{E}\mathcal{E}_2} A(\mathcal{E})}{\delta \mathcal{E}} B(\mathcal{E}_2) + A(\mathcal{E}) \frac{\delta_{\mathcal{E}\mathcal{E}_2} B(\mathcal{E})}{\delta \mathcal{E}} \right] \\ &= \frac{\delta_{\mathcal{E}\mathcal{E}_1\mathcal{E}_2}^2 A(\mathcal{E})}{\delta \mathcal{E}^2} B(\mathcal{E}_2) + \frac{\delta_{\mathcal{E}\mathcal{E}_1} A(\mathcal{E})}{\delta \mathcal{E}} \frac{\delta_{\mathcal{E}_1\mathcal{E}_2} B(\mathcal{E}_1)}{\delta \mathcal{E}_1} \\ &\quad + A(\mathcal{E}) \frac{\delta_{\mathcal{E}\mathcal{E}_1\mathcal{E}_2}^2 B(\mathcal{E})}{\delta \mathcal{E}^2}. \quad (\text{B2}) \end{aligned}$$

It should be noted that the operator $B(\mathcal{E}_2)$ is unaffected by the differentiation $\delta_{\mathcal{E}\mathcal{E}_1}$. Note also that, in view of the result (B1), the B operator in the second term of the last row depends on \mathcal{E}_1 . This result can be generalized to

$$\frac{\delta_{\mathcal{E}\mathcal{E}_1 \dots \mathcal{E}_n}^n}{\delta \mathcal{E}^n} [A(\mathcal{E}) B(\mathcal{E})] = \sum_{m=0}^n \frac{\delta_{\mathcal{E}\mathcal{E}_1 \dots \mathcal{E}_m}^m A(\mathcal{E})}{\delta \mathcal{E}^m} \frac{\delta_{\mathcal{E}_m \mathcal{E}_{(m+1)} \dots \mathcal{E}_n}^{(n-m)} B(\mathcal{E}_m)}{\delta \mathcal{E}_m^{(n-m)}} \quad (\text{B3})$$

(with $\varepsilon = \varepsilon_0$) or with simplified notations

$$\frac{\delta^n}{\delta \mathcal{E}^n} [A(\mathcal{E}) B(\mathcal{E})] = \sum_{m=0}^n \frac{\delta^m A(\mathcal{E})}{\delta \mathcal{E}^m} \frac{\delta^{(n-m)} B(\mathcal{E}_m)}{\delta \mathcal{E}_m^{(n-m)}}. \quad (\text{B4})$$

In the case of complete degeneracy we have in first-order

$$\lim_{\varepsilon_1 \rightarrow \mathcal{E}} \frac{\delta_{\varepsilon \varepsilon_1} A(\mathcal{E})}{\delta \mathcal{E}} = \frac{\partial A(\mathcal{E})}{\partial \mathcal{E}}, \quad (\text{B5})$$

while in second-order we have

$$\lim_{\varepsilon_1, \varepsilon_2 \rightarrow \mathcal{E}} \frac{\delta_{\varepsilon \varepsilon_1 \varepsilon_2}^2 A(\mathcal{E})}{\delta \mathcal{E}^2} = \frac{1}{2} \frac{\partial^2 A(\mathcal{E})}{\partial \mathcal{E}^2} \quad (\text{B6})$$

and generally

$$\lim_{\varepsilon_1, \varepsilon_2, \dots \rightarrow \mathcal{E}} \frac{\delta_{\varepsilon \varepsilon_1 \varepsilon_2}^n A(\mathcal{E})}{\delta \mathcal{E}^n} = \frac{1}{n!} \frac{\partial^n A(\mathcal{E})}{\partial \mathcal{E}^n}. \quad (\text{B7})$$

If we have a product of effective interactions, then they are separated by model-space states, which generally have different energies,

$$\dots P_2 V_{\text{eff}} P_1 V_{\text{eff}} P,$$

where P corresponds to the energy \mathcal{E} , P_1 to ε_1 , etc. This appears in multiple folded terms, and the effective interac-

tions have the corresponding energy parameter,

$$\dots P_2 V_{\text{eff}}(\varepsilon_1) P_1 V_{\text{eff}}(\mathcal{E}) P.$$

If we now form the difference ratio of this product

$$\frac{\delta}{\delta \mathcal{E}} [\dots P_2 V_{\text{eff}}(\varepsilon_1) P_1 V_{\text{eff}}(\mathcal{E}) P],$$

implying that the parameter \mathcal{E} is changed, only the last factor is affected, and

$$\frac{\delta}{\delta \mathcal{E}} [\dots P_2 V_{\text{eff}}(\varepsilon_1) P_1 V_{\text{eff}}(\mathcal{E}) P] = \dots P_2 V_{\text{eff}}(\varepsilon_1) P_1 \frac{\delta V_{\text{eff}}(\mathcal{E})}{\delta \mathcal{E}} P$$

or generally

$$\frac{\delta (V_{\text{eff}})^n}{\delta \mathcal{E}} = (V_{\text{eff}})^{(n-1)} \frac{\delta V_{\text{eff}}}{\delta \mathcal{E}}. \quad (\text{B8})$$

-
- [1] I. Lindgren and J. Morrison, *Atomic Many-Body Theory*, 2nd ed. (Springer-Verlag, Berlin, 1986).
- [2] I. Lindgren, *Mol. Phys.* **94**, 19 (1998).
- [3] I. Lindgren, B. Åsén, S. Salomonson, and A.-M. Mårtensson-Pendrill, *Phys. Rev. A* **64**, 062505 (2001).
- [4] I. Lindgren, S. Salomonson, and B. Åsén, *Phys. Rep.* **389**, 161 (2004).
- [5] I. Lindgren, S. Salomonson, and D. Hedendahl, *Can. J. Phys.* **83**, 183 (2005).
- [6] E. Lindroth and A. M. Mårtensson-Pendrill, *Phys. Rev. A* **39**, 3794 (1989).
- [7] G. E. Brown, *Philos. Mag.* **43**, 467 (1952).
- [8] M. H. Mittleman, *Phys. Rev. A* **5**, 2395 (1972).
- [9] P. Indelicato, *Phys. Rev. A* **51**, 1132 (1995).
- [10] I. Lindgren, H. Persson, S. Salomonson, and L. Labzowsky, *Phys. Rev. A* **51**, 1167 (1995).
- [11] P. J. Mohr, G. Plunien, and G. Soff, *Phys. Rep.* **293**, 227 (1998).
- [12] P. J. Mohr and J. Sapirstein, *Phys. Rev. A* **62**, 052501 (2000).
- [13] E. O. LeBigot, P. Indelicato, and V. M. Shabaev, *Phys. Rev. A* **63**, 040501(R) (2001).
- [14] V. M. Shabaev, *Phys. Rep.* **356**, 119 (2002).
- [15] A. N. Artemyev, V. M. Shabaev, V. A. Yerokhin, G. Plunien, and G. Soff, *Phys. Rev. A* **71**, 062104 (2005).
- [16] G. W. F. Drake, *Phys. Rev. A* **19**, 1387 (1979).
- [17] G. W. F. Drake, *Can. J. Phys.* **66**, 586 (1988).
- [18] G. W. F. Drake, *Can. J. Phys.* **80**, 1195 (2002).
- [19] K. Pachucki, *J. Phys. B* **35**, 13087 (2002).
- [20] K. Pachucki and J. Sapirstein, *J. Phys. B* **35**, 1783 (2002).
- [21] J. Sucher, *Phys. Rev.* **109**, 1010 (1957).
- [22] M. H. Douglas and N. M. Kroll, *Ann. Phys.* **82**, 89 (1974).
- [23] M. C. George, L. D. Lombardi, and E. A. Hessels, *Phys. Rev. Lett.* **87**, 173002 (2001).
- [24] P. C. Pastor, G. Giusfredi, P. DeNatale, G. Hagel, C. deMauro, and M. Inguscio, *Phys. Rev. Lett.* **92**, 023001 (2004).
- [25] T. Zelevinsky, D. Farkas, and G. Gabrielse, *Phys. Rev. Lett.* **95**, 203001 (2005).
- [26] P. Mohr and B. Taylor, *Rev. Mod. Phys.* **77**, 1 (2005).
- [27] S. Fritzsche, P. Indelicato, and T. Stöhlker, *J. Phys. B* **38**, S707 (2005).
- [28] D. Hedendahl, S. Salomonson, and I. Lindgren (unpublished).
- [29] I. Lindgren, *J. Phys. B* **7**, 2441 (1974).
- [30] C. Bloch, *Nucl. Phys.* **6**, 329 (1958).
- [31] C. Bloch, *Nucl. Phys.* **7**, 451 (1958).
- [32] I. Lindgren, *Int. J. Quantum Chem.* **S12**, 33 (1978).
- [33] A. L. Fetter and J. D. Walecka, *The Quantum Mechanics of Many-Body Systems* (McGraw-Hill, New York, 1971).
- [34] M. Gell-Mann and F. Low, *Phys. Rev.* **84**, 350 (1951).
- [35] J. Goldstone, *Proc. R. Soc. London, Ser. A* **239**, 267 (1957).
- [36] T. T. S. Kuo and G. E. Brown, *Nucl. Phys.* **85**, 40 (1966).
- [37] S. S. Schweber, *An Introduction to Relativistic Quantum Field Theory* (Harper and Row, New York, 1961).
- [38] A.-M. Mårtensson, *J. Phys. B* **12**, 3995 (1980).
- [39] I. Lindgren, *Phys. Rev. A* **31**, 1273 (1985).
- [40] E. Lindroth, *Phys. Rev. A* **37**, 316 (1988).
- [41] S. Salomonson and P. Öster, *Phys. Rev. A* **41**, 4670 (1989).
- [42] S. Salomonson and A. Ynnerman, *Phys. Rev. A* **43**, 88 (1991).
- [43] S. Salomonson and P. Öster, *Phys. Rev. A* **40**, 5548 (1989).
- [44] S. Salomonson and P. Öster, *Phys. Rev. A* **40**, 5559 (1989).
- [45] B. Åsén, S. Salomonson, and I. Lindgren, *Phys. Rev. A* **65**, 032516 (2002).
- [46] A. R. Edmonds, *Angular Momentum in Quantum Mechanics* (Princeton University Press, Princeton, New Jersey, 1957).
- [47] I. Lindgren and A. Rosén, *Case Stud. At. Phys.* **4**, 93 (1974).
- [48] G. Arfken, *Mathematical Methods for Physicists* (Academic, San Diego, 1985).