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Energy-dependent many-body perturbation theory: A road towards a Many-Body-QED Procedure.

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A rigorous procedure for energy-dependent many-body perturbation theory (MBPT) is presented. This can be applied for numerical evaluation of many-body-QED effects by combining QED with electron correlation to arbitrary order. So far, it has been used only for the exchange of a single retarded photon together with an arbitrary number of instantaneous Coulomb interactions. For heliumlike neon this represents more than 99 % of the nonradiative effect on the energy beyond standard MBPT.

1. Introduction

The standard procedure for time- or energy-independent many-body perturbations on atomic, molecular and nuclear systems, normally referred to as the *Many-Body Perturbation Theory* (MBPT), is well developed [1]. It is capable of handling electron correlation essentially to all orders and it can deal with the quasidegeneracy problem by means of the procedure with *extended model space*. This is indicated in the second line of the table below. There we also have indicated that the S-matrix formalism can handle QED problems but neither electron correlation nor quasidegeneracy. Two methods are available that can deal with QED as well as quasidegeneracy, namely the *two-times Green's-function* method of Shabaev *et al.* [2] and the *Covariant-Evolution-Operator* method, recently introduced by us [4,3], as indicated in the next line of the table.

Electron correlation	**Quasi-degeneracy**	**Q E D**
Std. M B P T		**S-matrix**
	Two-times Green's function Cov. Evol. Oper. method	
MANY-BODY Cov. Evol. Oper. method		

All numerical QED procedures presently available are of independent-particle type, where the electrons move independently of each other in some average (usually nuclear) field and interact by the exchange of one or two covariant photons. This implies that the many-body effect (electron correlation) is treated at most to second order by these methods, which is often insufficient in interpreting heavy-ion experiments [5]. (An approximate scheme for combining QED effects with higher-order electron correlation, based upon the $1/Z$ expansion, has recently been developed by Shabaev et al. [6].)

As the accuracy of heavy-ion experiments improve, the many-body effects become even more important, and it is desirable to be able to include these effects in a systematic fashion. It turns out that the Covariant-Evolution-Operator method has a structure that is quite similar to standard MBPT, which opens up the possibility of combining the two procedures, so that they can form a true "*Many-Body-QED*" procedure. We have indicated this possibility previously [3] and developed this further in a more recent publication [7]. We refer to this new method as the *Many-Body Covariant-Evolution-Operator* method, indicated in the last line of the table. In the present paper we shall analyze this procedure further and compare it with other available procedures.

The most accurate method now available for QED calculations on light elements is the analytical method, developed and applied by Drake, Pachucki and others [8,9,10,11]. This is based upon a perturbative expansion of the relativistic and QED effects and therefore yields limited accuracy of heavier elements. We believe that the numerical method proposed here could be a complement to the analytical one.

2. Standard Time-independent Many-Body Perturbation Theory

In standard time-independent many-body perturbation theory [1] we consider a number of *target states*, Ψ^α, satisfying the time-independent Schrödinger equation

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

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

$$H = H_0 + H'. \tag{2}$$

The Hilbert space formed by the eigenstates of H_0 is separated into a *model space* (P), containing all eigenstates corresponding to one or several eigenvalues of H_0, and a *complementary space* (Q). For each target state there is a *model state*, which in the *intermediate normalization* is the projection onto the model space of the corresponding target state,

$$\Psi_0^\alpha = P\Psi^\alpha. \tag{3}$$

A *wave operator* transforms the model states to the corresponding target states

$$\Psi^\alpha = \Omega\,\Psi_0^\alpha. \tag{4}$$

An *effective Hamiltonian*

$$H_{\rm eff} = PH\Omega P = PH_0P + PH'\Omega P = PH_0P + V_{\rm eff} \tag{5}$$

satisfies the secular equation

$$H_{\rm eff}\,\Psi_0^\alpha = E^\alpha\,\Psi_0^\alpha. \tag{6}$$

$V_{\rm eff}$ is known as the *effective interaction*.

The wave operator satisfies the generalized Bloch equation [12,13,14,1]

$$\boxed{\big[\Omega, H_0\big]P = \big(H'\Omega - \Omega\,V_{\rm eff}\big)P} \tag{7}$$

which leads to the generalized Rayleigh-Schrödinger perturbation expansion. Expressed in terms of Goldstone diagrams, this leads to the Brueckner-Goldstone [15,16] linked-diagram expansion

$$\boxed{\big[\Omega, H_0\big]P = \big(H'\Omega - \Omega\,V_{\rm eff}\big)_{\rm linked}P} \tag{8}$$

where all terms on the right-hand side are *"linked"*. Separating the second-quantized wave operator in terms of one-, two-, ... body parts, leads to a system of coupled equations, and solving these self-consistently yields the corresponding correlation effects to essentially *all orders* of perturbation theory. The normal-ordered exponential Ansatz, $\Omega = \{{\rm e}^S\}$, leads similarly to the very effective *Coupled-Cluster Approach* (CCA) [1,17].

The important point here is that the commutator of the left-hand side makes the equations applicable also to a model space that contains several unperturbed energies. This so-called *extended-model-space procedure* is very effective in dealing with near or *quasidegeneracy*.

3. S-matrix formalism and covariant-evolution operator method

3.1. *Time-evolution operator*

We employ the *interaction picture*, where the wave functions and the operators are related to those of the Schrödinger picture by

$$\Psi_{\rm I}(t) = {\rm e}^{{\rm i}H_0t}\Psi_{\rm S}(t)\,; \qquad O_{\rm I}(t) = {\rm e}^{{\rm i}H_0t}O_{\rm S}\,{\rm e}^{-{\rm i}H_0t}. \tag{9}$$

The perturbation is assumed to be the interaction between the electrons and the electromagnetic radiation field

$$\mathcal{H}'_{\rm I}(x) = -e\hat{\psi}^\dagger_{\rm I}\alpha^\mu A_\mu \hat{\psi}_{\rm I}, \tag{10}$$

where $\hat{\psi}_{\rm I}$, $\hat{\psi}^\dagger_{\rm I}$ are the electron field operators, α^μ the Dirac alpha operators and A_μ represents the radiation field. We also employ the *adiabatic damping*, implying that

$$H'_{\rm I}(t) \to H'_{{\rm I}\gamma}(t) = H'_{\rm I}(t)\,{\rm e}^{-\gamma|t|}, \tag{11}$$

where γ is a small, positive number, which eventually goes to zero. The time-evolution operator is in this picture defined by

$$\Psi_{{\rm I}\gamma}(t) = U_\gamma(t,t_0)\,\Psi_{{\rm I}\gamma}(t_0) \tag{12}$$

and can be expressed as the expansion [18]

$$U_\gamma(t,t_0) = 1 + \sum_{n=1}^{\infty}\frac{(-{\rm i})^n}{n!}\int_{t_0}^{t}{\rm d}^4x_n\cdots\int_{t_0}^{t}{\rm d}^4x_1\;T_{\rm D}\big[\mathcal{H}'_{\rm I}(x_n)\mathcal{H}'_{\rm I}(x_{n-1})\cdots\mathcal{H}'_{\rm I}(x_1)\big] \times {\rm e}^{-\gamma(|t_1|+\cdots+|t_n|)}. \tag{13}$$

$T_{\rm D}$ is the Dyson time-ordering operator, and $\mathcal{H}'_{\rm I}(x)$ is the perturbation *density*

$$H'_{\rm I}(t) = \int {\rm d}^3\boldsymbol{x}\,\mathcal{H}'_{\rm I}(t,\boldsymbol{x}). \tag{14}$$

3.2. *Gell-Mann–Low theorem and the reduced evolution operator*

According to the Gell-Mann-Low theorem [19], the time-independent wave function can in the single-reference case (one-dimensional model space) be expressed

$$\Psi = \lim_{\gamma\to 0}\Psi_{{\rm I}\gamma}(t=0) = \lim_{\gamma\to 0}\frac{U_\gamma(0,-\infty)\Psi_0}{\langle\Psi_0|U_\gamma(0,-\infty)\,|\Psi_0\rangle}, \tag{15}$$

satisfying the time-independent Schrödinger equation

$$\big(H_0 + H'\big)\,\Psi = E\,\Psi, \tag{16}$$

provided that the undamped perturbation H' is time-independent in the Schrödinger picture. The evolution operator generally becomes singular as $\gamma\to 0$, but these singularities are eliminated in the ratio (15). The energy eigenvalue is given by $E = E_0 + \Delta E$ with

$$\Delta E = \lim_{\gamma\to 0}{\rm i}\gamma\lambda\,\frac{\langle\Psi_0|\frac{\partial}{\partial\lambda}U_\gamma(0,-\infty|\Psi_0\rangle}{\langle\Psi_0|U_\gamma(0,-\infty|\Psi_0\rangle}. \tag{17}$$

(Here, the Hamiltonian is temporarily expressed $H = H_0 + \lambda H'$ with λ eventually set equal to unity.)

The GML theorem can be extended to the multi-reference case [3], yielding

$$\Psi^\alpha = \lim_{\gamma\to 0}\frac{N^\alpha\,U_\gamma(0,-\infty)\,\Phi^\alpha}{\langle\Phi^\alpha|U_\gamma(0,-\infty)|\Phi^\alpha\rangle}. \tag{18}$$

N^α is a normalization constant and Φ^α is the *parent state*

$$\Phi^\alpha = \lim_{\gamma\to 0}\lim_{t\to-\infty} \Psi^\alpha_{\mathrm{I}\gamma}(t). \tag{19}$$

The evolution operator can generally be expressed

$$U_\gamma(t,-\infty)P = P + \widetilde{U}_\gamma(t,-\infty)PU_\gamma(0,-\infty)P, \tag{20}$$

where $\widetilde{U}_\gamma(t,-\infty)$, known as the *reduced evolution operator*, is regular [4]. This leads to the *factorization theorem*

$$U_\gamma(0,-\infty)P = \left[1 + Q\widetilde{U}_\gamma(0,-\infty)\right] PU_\gamma(0,-\infty)P, \tag{21}$$

which together with the Gell-Mann–Low theorem (15) yields the important relation between the evolution operator and the wave operator (4)

$$\boxed{Q\Omega P = Q\widetilde{U}(0,-\infty)P} \tag{22}$$

The effective interaction (5) is related to the evolution operator by [3]

$$\boxed{V_{\mathrm{eff}} = P\Big[\mathrm{i}\frac{\partial}{\partial t}\widetilde{U}(t,-\infty)\Big]_{t=0}P.} \tag{23}$$

These relations give the connection between the covariant-evolution-operator method and standard MBPT.

3.3. *Single-photon exchange*

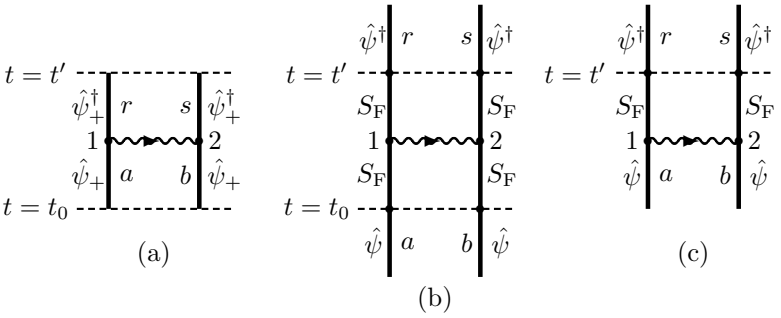

Fig. 1. Graphical representation of the standard evolution operator for single-photon exchange (a). This can be made covariant by inserting electron propagators (S_{F}) or zeroth-order Green's functions on the in- and outgoing states (b). This can be simplified by letting $t_0 \to -\infty$ (c). The wavy lines represent covariant photons, and the free vertical lines single-electron states in the bound-interaction picture (28), while the internal lines between heavy dots represent the corresponding electron propagators.

The evolution operator (13) for single-photon exchange (Fig. 1 a) is

$$U^{(2)}_\gamma(t',t_0) = -\frac{1}{2}\iint_{t_0}^{t'} \mathrm{d}^4x_1\mathrm{d}^4x_2\, \hat{\psi}^\dagger_{\mathrm{I}+}(x_1)\hat{\psi}^\dagger_{\mathrm{I}+}(x_2)\, \mathrm{i}I(x_1,x_2)\, \hat{\psi}_{\mathrm{I}+}(x_2)\hat{\psi}_{\mathrm{I}+}(x_1)\, \mathrm{e}^{-\gamma(|t_1|+|t_2|)}, \tag{24}$$

integrated over all space and over time as indicated. $\hat{\psi}_{\rm I+}$, $\hat{\psi}^\dagger_{\rm I+}$ are the positive-energy parts of the electron-field operators, and

$$\mathrm{i}I(x_1,x_2) = (-e\alpha^\mu \overbrace{A_\mu)_1(-e\alpha^\nu A}_\nu)_2 = e^2\alpha_1^\mu\alpha_2^\nu\,\mathrm{i}D_{F\mu\nu}(x_1-x_2). \tag{25}$$

The hook represents contraction between the photon operators, and $D_{\mathrm{F}\mu\nu}(x_1-x_2)$ is the Feynman *photon propagator*. Integration over all times yields the corresponding *S-matrix*

$$S^{(2)}_\gamma = -\frac{1}{2}\iint_{-\infty}^{\infty} \mathrm{d}^4x_1\mathrm{d}^4x_2\,\hat{\psi}^\dagger_{\rm I+}(x_1)\hat{\psi}^\dagger_{\rm I+}(x_2)\,\mathrm{i}I(x_1,x_2)\,\hat{\psi}_{\rm I+}(x_2)\hat{\psi}_{\rm I+}(x_1)\,\mathrm{e}^{-\gamma(|t_1|+|t_2|)}. \tag{26}$$

The matrix elements of the S-matrix become in the limit $\gamma\to 0$

$$\left\langle rs\left|S^{(2)}\right|ab\right\rangle = -2\pi\mathrm{i}\,\delta(q+q')\,\langle rs|I(\boldsymbol{x}_1,\boldsymbol{x}_2,q)|ab\rangle, \tag{27}$$

where $I(\boldsymbol{x}_1,\boldsymbol{x}_2,q)$ is the Fourier transform of the interaction (25). $r,s...$ represent single-electron states, generated by solving the Dirac equation in the nuclear field

$$h_{\rm D}|i\rangle = \varepsilon_i|i\rangle, \tag{28}$$

and $q=\varepsilon_a-\varepsilon_r$ and $q'=\varepsilon_b-\varepsilon_s$ are the negative single-electron excitation energies. The S-matrix elements become singular, when the energy conservation criterion

$$q+q' = \varepsilon_a+\varepsilon_b-\varepsilon_r-\varepsilon_s = 0 \tag{29}$$

is satisfied and zero otherwise. The corresponding energy contribution is given by the Sucher formula [20]

$$\Delta E = \lim_{\gamma\to 0}\frac{\mathrm{i}}{2}\gamma\lambda\,\frac{\langle\Psi_0|\frac{\partial}{\partial\lambda}S_\gamma|\Psi_0\rangle}{\langle\Psi_0|S_\gamma|\Psi_0\rangle}\,, \tag{30}$$

which in this case yields

$$\Delta E = \delta_{q,-q'}\,\big\langle rs\big|I(\boldsymbol{x}_1,\boldsymbol{x}_2,q)\big|ab\big\rangle, \tag{31}$$

$\delta_{x,y}$ being the Kronecker delta. This is non-zero only when the energy (29) is conserved. The integration kernel is

$$I(\boldsymbol{x}_1,\boldsymbol{x}_2,q) = \int_0^\infty \frac{2k\,\mathrm{d}k\,f(\boldsymbol{x}_1,\boldsymbol{x}_2,k)}{q^2-k^2+\mathrm{i}\eta} \tag{32}$$

where $f(\boldsymbol{x}_1,\boldsymbol{x}_2,k)$ is a gauge-dependent function of the photon momentum. The energy conservation (29) restricts the S-matrix application to cases with a one-dimensional or a completely degenerate model space, preventing the application to quasidegenerate systems.

The evolution operator (24) is *non-covariant* for finite times, but it can be made covariant by integrating over *all* times, which yields the S matrix (26). Alternatively, it can be made covariant by inserting zeroth-order Green's functions on the in- and outgoing states [3] (see Fig. 1 b)

$$U^{(2)}_{\gamma\mathrm{Cov}}(t',t_0) = -\frac{1}{2}\iint \mathrm{d}^3\boldsymbol{x}'_1\mathrm{d}^3\boldsymbol{x}'_2\,\hat{\psi}^\dagger_{\rm I}(x'_1)\hat{\psi}^\dagger_{\rm I}(x'_2)\iint \mathrm{d}^4x_1\mathrm{d}^4x_2\,G_0(x'_1,x'_2;x_1,x_2)$$
$$\times\iint \mathrm{d}^3\boldsymbol{x}_{10}\mathrm{d}^3\boldsymbol{x}_{20}\,\mathrm{i}I(x_1,x_2)\,G_0(x_1,x_2;x_{10},x_{20})\,\hat{\psi}_{\rm I}(x_{20})\hat{\psi}_{\rm I}(x_{10})\,\mathrm{e}^{-\gamma(|t_1|+|t_2|)} \tag{33}$$

and performing the time integrations of t_1 and t_2 over *all times*. The initial and final times can still be finite and are the same for all electrons, i.e.,

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

Starting the perturbation from unperturbed states, we can set the initial time $t_0 = -\infty$, and the expression is simplified to

$$U^{(2)}_{\gamma\mathrm{Cov}}(t', -\infty) = \frac{1}{2} \iint \mathrm{d}^3\boldsymbol{x}'_1 \mathrm{d}^3\boldsymbol{x}'_2 \, \hat{\psi}^\dagger_{\mathrm{I}}(x'_1)\hat{\psi}^\dagger_{\mathrm{I}}(x'_2) \iint \mathrm{d}^4x_1 \mathrm{d}^4x_2 \, G_0(x'_1, x'_2; x_1, x_2) \times \mathrm{i}I(x_1, x_2) \, \hat{\psi}_{\mathrm{I}}(x_2)\hat{\psi}_{\mathrm{I}}(x_1) \, \mathrm{e}^{-\gamma(|t_1|+|t_2|)} \tag{35}$$

(see Fig. 1 c). This yields in the limit $\gamma \to 0$ the matrix element for single-photon exchange

$$\Big\langle rs \Big| U^{(2)}_{\mathrm{Cov}}(t', -\infty) \Big| ab \Big\rangle = \frac{\mathrm{e}^{-\mathrm{i}t'(q+q')}}{q+q'} \, \big\langle rs \big| I(\boldsymbol{x}_1, \boldsymbol{x}_2, q, q') \big| ab \big\rangle, \tag{36}$$

with

$$I(\boldsymbol{x}_1, \boldsymbol{x}_2, q, q') = \int \mathrm{d}k \, f(\boldsymbol{x}_1, \boldsymbol{x}_2, k) \Big[\frac{1}{q - (k - \mathrm{i}\eta)_r} + \frac{1}{q' - (k - \mathrm{i}\eta)_s} \Big], \tag{37}$$

where $(A)_x = A \, \mathrm{sgn}(\varepsilon_x)$. In this order $Q\widetilde{U}^{(2)}_{\mathrm{Cov}}(t, -\infty)P = QU^{(2)}_{\mathrm{Cov}}(t, -\infty)P$, and the corresponding contribution to the wave operator (22) becomes

$$\langle rs \, |\Omega| \, ab \rangle = \frac{1}{q+q'} \, \big\langle rs \big| I(\boldsymbol{x}_1, \boldsymbol{x}_2, q, q') \big| ab \big\rangle \qquad (|rs\rangle \in Q) \tag{38}$$

and to the effective interaction (23)

$$\langle rs \, |V_{\mathrm{eff}}| \, ab \rangle = \big\langle rs \big| I(\boldsymbol{x}_1, \boldsymbol{x}_2, q, q') \big| ab \big\rangle \qquad (|rs\rangle \in P). \tag{39}$$

In the case of energy conservation (29) we find that the last expression becomes identical to the S-matrix result (31).

In the evolution-operator case (39) there is no energy restriction, which implies that also non-diagonal elements of the effective Hamiltonian (5) can be evaluated, and the procedure with extended model space can be applied in order to treat quasidegeneracy. As mentioned, in the S-matrix formalism this is not possible due to the energy restriction (29). An important relation is also the wave-operator expression (38), which gives the connection to the wave function. This has no counterpart in the S-matrix formalism.

4. Many-Body Covariant-Evolution-Operator Approach: Including electron correlation

Presently available methods for bound.state-QED calculations are essentially independent-particle models, based upon electrons moving independently of each other in some average field (usually the nuclear field) and interact with each other by exchanging covariant photons. No other many-body effects are included, i.e., no electron correlation apart from that represented by the covariant photons. Since at

most two such photons can be handle computationally at present, this implies that the many-body effects are poorly treated.

In the present paper we shall briefly describe how the covariant-evolution-operator method can be extended to include electron-correlation effects to arbitrary order of perturbation theory and hence forming a true many-body-QED procedure. (For more details the reader is referred to our recent publication [7].)

The retarded interaction (25) is the result of *two* perturbations (10)—the emission and the absorption of a virtual photon at different times. Here, we consider each of them as individual perturbations in the Gell-Mann–Low relations (15, 18). The wave functions will then lie in an *extended Fock space*, where the number of photons is no longer conserved, and we express the Schrödinger-like equation (16) as

$$\big(\boldsymbol{H}_0 + H'\big)\,\boldsymbol{\Psi} = E\,\boldsymbol{\Psi}, \tag{40}$$

indicating with the bold symbols quantities lying in the extended space ($\boldsymbol{H}_0$ contains also the photon field.) This leads to a Bloch equation, analogous to the standard one (7),

$$\boxed{\big[\boldsymbol{\Omega}, \boldsymbol{H}_0\big]P = \big(H'\boldsymbol{\Omega} - \boldsymbol{\Omega}\,V_{\rm eff}\big)P} \tag{41}$$

which we can solve in a step-by-step process.

We employ the *Coulomb gauge*, where the interaction between the electrons consists of the instantaneous Coulomb interaction $V_{12} = \frac{e^2}{4\pi r_{12}}$ and the retarded Breit interaction. The latter is represented by the expression (37) with

$$f(\boldsymbol{x}_1, \boldsymbol{x}_2, k) = \frac{e^2}{4\pi^2}\Big[- \boldsymbol{\alpha_1}\cdot\boldsymbol{\alpha_2}\frac{\sin(kr_{12})}{r_{12}} + (\boldsymbol{\alpha_1}\cdot\boldsymbol{\nabla_1})\,(\boldsymbol{\alpha_2}\cdot\boldsymbol{\nabla_2})\frac{\sin(kr_{12})}{k^2\,r_{12}}\Big], \tag{42}$$

r_{12} being the interelectronic distance. The first term represents the Gaunt interaction and the second term the scalar-retardation part. By means of the expansion theorem

$$\frac{\sin(kr_{12})}{kr_{12}} = \sum_{l=0}^{\infty}(2l+1)j_l(kr_1)j_l(kr_2)\boldsymbol{C}^l(1)\cdot\boldsymbol{C}^l(2), \tag{43}$$

where $\boldsymbol{C}$ is a spherical tensor of rank l and j_l is a spherical Bessel function, we can express the relation (42) as [7]

$$f(\boldsymbol{x}_1, \boldsymbol{x}_2, k) = \sum_{l=0}^{\infty}\Big[- V_G^l(kr_1)\cdot V_G^l(kr_2) + V_{\rm SR}^l(kr_1)\cdot V_{\rm SR}^l(kr_2)\Big]. \tag{44}$$

In this way we have separated the Gaunt and the scalar-retardation parts of the retarded interaction into products of single-particle operators, and we can regard each of them as the perturbation in the Schrödinger-like equation (40) and the Bloch equation (41).

By first applying the instantaneous Coulomb interaction, V_{12}, we have the standard Bloch equation, for a two-electron system leading to the standard pair equation

$$\big(\varepsilon_a + \varepsilon_b - h_0(1) - h_0(2)\big)|\rho_{ab}\rangle = |rs\rangle\langle rs|V_{12}|\rho_{ab}\rangle - |\rho_{cd}\rangle\langle cd|V_{\rm eff}|ab\rangle. \tag{45}$$

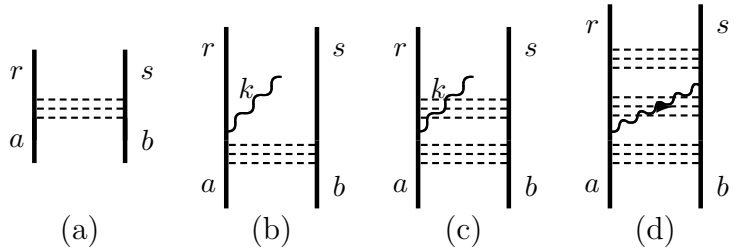

Fig. 2. Illustrations of solving the extended Bloch equation (41) step by step, leaving out the folded terms.

The pair function ρ_{ab} is illustrated in Fig. 2 (a). The last term of the equation represents the folded term, which is not shown in the figure.

In the next step we apply one of the retarded interactions, leading to a function with one extra photon and to the pair equation

$$\big(\varepsilon_a + \varepsilon_b - h_0(1) - h_0(2) - k\big)|\rho^l_{\mathrm{G},ab}(k)\rangle = |rs\rangle\langle rs|V^l_G(k)|\rho_{ab}\rangle - |\rho^l_{\mathrm{G},cd}(k)\rangle\langle cd|V_{\mathrm{eff}}|ab\rangle, \quad (46)$$

illustrated in Fig. 2 (b). The last term represents a new type of folded diagram (also not shown in the figure). Before the photon is being absorbed, we can have additional Coulomb interactions,

$$\begin{aligned}\big(\varepsilon_a + \varepsilon_b - h_0(1) - h_0(2) - k\big)|\rho^l_{\mathrm{G},ab}(k)\rangle &= |rs\rangle\langle rs|V^l_G(k)|\rho_{ab}\rangle + |rs\rangle\langle rs|V_{12}|\rho^l_{\mathrm{G},ab}(k)\rangle \\ &\quad - |\rho^l_{\mathrm{G},cd}(k)\rangle\langle cd|V_{\mathrm{eff}}|ab\rangle, \quad (47)\end{aligned}$$

as illustrated in Fig. 2 (c).

Finally, the photon is absorbed and additional Coulomb interactions added,

$$\begin{aligned}\big(\varepsilon_a + \varepsilon_b - h_0(1) - h_0(2)\big)|\rho_{\mathrm{G},ab}\rangle &= |rs\rangle\langle rs|V^l_G(k)|\rho^l_{\mathrm{G},ab}(k)\rangle + |rs\rangle\langle rs|V_{12}|\rho_{\mathrm{G},ab}\rangle \\ &\quad - |\rho_{G,cd}\rangle\langle cd|V_{\mathrm{eff}}|ab\rangle, \quad (48)\end{aligned}$$

as illustrated in Fig. 2 (d).

We have here illustrated the procedure by the exchange of a photon *between* two electrons. The same procedure can be used also when the photon is absorbed by *the same* electron, leading to radiative effects, like the self-energy and vertex correction—of course, with the proper renormalization.

5. Numerical results

In Fig. 3 we have illustrated our preliminary numerical results for the $1s2s\,{}^1S$ state of heliumlike neon. (a) represents the effect of the exchange of one retarded photon, (b) the effect of one retarded photon with one noncrossing Coulomb interaction and (c) with one crossing, (d) the effect of two retarded photons (crossing and noncrossing), (e) the effect of one retarded photon with preceding and succeeding Coulomb interactions, (f) the same with crossing Coulomb interactions, and (g) the effect of two retarded photons with electron correlation. The results (c, d) are

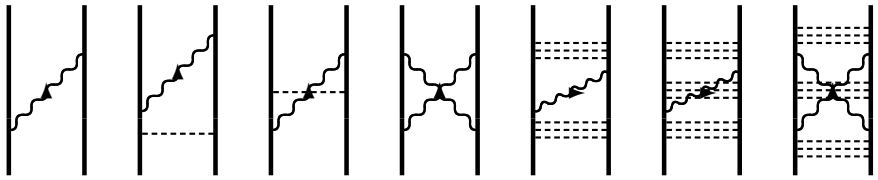

Fig. 3. Numerical results for the energy of the $1s2s\,^1S$ state of heliumlike neon. The diagrams (c, d) are taken from our previous work and (f, g) are estimated. The diagrams (a-d) can evaluated by the standard QED techniques and (e, f) with the new technique presented here.

taken from our previous S-matrix calculation [21]. The main new result of the work presented here is represented by the many-body-QED diagrams (e, f), which have substantial effect. (The result (f) is only estimated—numerical evaluation is underway.) The diagram (g) is presently beyond reach and has been estimated. In the standard QED procedures the effects (a-d) can be evaluated, which in the present case corresponds to 97 % of the energy contribution beyond standard MBPT. With the new procedure discussed here the effects (a-f) can be evaluated, corresponding to 99.9 % of this energy.

6. Summary and Conclusions

We have presented a rigorous Many-Body-QED scheme, where QED effects are combined with electron correlation to arbitrary order. We have here considered only a single retarded photon and an arbitrary number of instantaneous Coulomb interactions. This can be repeated, leading to *reducible* diagrams with the retarded interactions separated in time. In principle, the procedure can be used also for several *irreducible* photons, i.e., photons overlapping in time, although this is considerably more time consuming computationally. Our preliminary numerical results indicate [7] that for light and medium-heavy elements the effect of the combination of a single retarded photon and electron correlation beyond second order is much more important than the effect of two retarded photons. (To treat three retarded photons numerically is presently beyond reach computationally.) Therefore, the proposed scheme seems to represent the most efficient way of improving the numerical QED calculations on such systems, and we believe that the method—after further refinements—could be a valuable complement to the analytical method, also for light elements.

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