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Treatment of Atomic Quasi-degeneracy in Bound-state QED. Application to the $1s2p$ States of He-like Ions.

Ingvar Lindgren, Ann-Marie Mårtensson-Pendrill, Sten Salomonson,
and Björn Åsén
Department of Physics, Chalmers University of Technology
and Göteborg University, SE-412 96 Göteborg, Sweden

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Abstract

In the case of quasi-degeneracy, i.e., when there are states close in energy to the state considered, standard perturbation theory may lead to convergence problem. A typical example is the relativistic treatment of the fine structure of light heliumlike ions. In Many-Body-Perturbation Theory (MBPT) this problem can be treated by including the quasi-degenerate states in an extended model space. The mixing is then treated to all orders already in the zeroth-order wave function by diagonalizing an effective hamiltonian in this subspace. Only non-quasi-degenerate states are treated by perturbation.

Standard QED treatment of bound systems is based upon the S-matrix formalism. Here an extended model space cannot be used, the reason being that only matrix elements diagonal in energy can be determined, while the effective hamiltonian needed contains also non-diagonal elements between the states in the model space. In the present paper a modification of the bound-state QED procedure is described, based upon a covariant form of the time-evolution operator, rather than the S-matrix. In this way also elements non-diagonal in energy can be evaluated. The operator appearing in the final procedure is free from singularities, and no special procedure is needed for evaluating the so-called *Model-Space Contribution*, caused by model-space states appearing as the intermediate states.

The procedure has been applied to the fine structure of helium-like ions, and numerical second-order QED results, including quasi-degenerate levels, are presented for the first time. The formalism is closely related to MBPT and may open the possibility to combine QED and MBPT in a more systematic fashion.

Introduction

During the last decade there has been increasing interest in bound-state quantum-electro-dynamical (QED) calculations on highly charged ions, mainly due to the advent of new experimental techniques, such as storage rings and ion traps, and the simultaneous development of the computational technique. It is now possible to study such systems with high experimental accuracy, and the comparison with accurate numerical calculations can be seen as a test of QED at strong-fields.

The bound-state QED calculations are normally based upon the *S-matrix* formalism and the adiabatic limiting process of Gell-Mann–Low[1] and Sucher [2], a procedure with certain limitations. Most importantly, in this procedure only matrix elements *diagonal in energy* can be obtained, which implies that it cannot be applied to an *extended model space* with several (quasi-degenerate) eigenvalues.

A good example of quasi-degeneracy is the fine-structure of light heliumlike ions. In, for instance, the $1s2p$ multiplet of these ions there are two states with total $J = 1$, which are mixtures of the jj-coupled states $1s2p_{1/2}$ and $1s2p_{3/2}$. In a relativistic many-body treatment these states are strongly mixed, due to the proximity in energy for low Z, and in a conventional perturbation expansion one has encounted severe convergence problems [3]. By working with an extended model space, containing the quasi-degenerate states, we have shown previously that the convergence problems disappear [4].

In order to apply a similar technique in bound-state QED, it is necessary to find a procedure that makes it possible to evaluate also elements non-diagonal in energy of the effective hamiltonian. Such a technique, based upon the *covariant form of the time-evolution operator*, has recently been presented [5] and is briefly described in the present paper. It gives the same results as the standard technique for diagonal elements but can in addition yield off-diagonal elements. Second-order numerical results for the fine structure of some heliumlike ions, incluing quasi-degenerate levels, are given here for the first time. More details will be given in a forthcoming paper.

In principle, quasi-degeneracy can also be handled by means of the so-called *two-times Green's-function* technique, developed in particular by Shabaev and coworkers [6, 7]. As a matter of fact, the two methods are closely related [5]. We believe, however, that the evolution-operator technique is easier to handle in practical work. To our knowledge no numerical results for the energy shifts of a quasi-degenerate system due to QED beyond first order have to date been presented [1].

Many-Body Perturbation Theory

As an introduction we give here a short summary of the MBPT for an extended model space. We partition the full hamiltonian in the standard way into a zeroth-order part and a perturbation, $H = H_0 + H'$. In standard perturbation theory the second-order energy contribution to the unperturbed state $|\Phi_a\rangle$ is then given by

$$E^{(2)} = \sum_{i \neq a} \frac{\langle \Phi_a | H' | \Phi_i \rangle \langle \Phi_i | H' | \Phi_a \rangle}{E_0^a - E_0^i}. \tag{1}$$

Φ_i is an eigenstate of the unperturbed hamiltonian, H_0, with the eigenvalue E_0^i. In the case of quasi-degeneracy some of the energy denominators become very small, which can lead to convergence problems in the traditional perturbation treatment, using a single reference function [3]. In more refined MBPT it is possible to work with several reference functions, based on an *effective hamiltonian*, H_{eff}, and an *extended model space* [4, 9, 10]. This leads to the secular equation

$$H_{\text{eff}} |\Psi_0^\alpha\rangle = E^\alpha |\Psi_0^\alpha\rangle \tag{2}$$

to be solved within the model space. The eigenvalues of the effective hamiltonian are the exact energies, E^α, of the system, although this operates only within the model space. The eigenvectors are the *correct zeroth-order functions* (ZOF), $|\Psi_0^\alpha\rangle$, corresponding to the exact states, $|\Psi^\alpha\rangle$.

After diagonalizing the effective hamiltonian, the full wave functions, $|\Psi^\alpha\rangle$, can be constructed from the ZOF's by means of the *wave operator* or *Møller operator* [10], Ω,

$$|\Psi^\alpha\rangle = \Omega |\Psi_0^\alpha\rangle, \tag{3}$$

satisfying the so-called *generalized Bloch equation* [9, 10, 11]

$$[\Omega, H_0] P = (H' \Omega - \Omega H'_{\text{eff}}) P. \tag{4}$$

[1] The contribution to the effective hamiltonian for quasi-degenerate systems due to the screened vacuum polarization together with the first-order electron-electron interaction have recently been published [8], and similar calculations for the screened self energy are under way in Paris, as reported by P. Indelicato and É.-O. Le Bigot at this workshop

Here, H'_{eff} is the *effective perturbation*, related to the full effective hamiltonian by $H_{\rm eff} = PH_0P + H'_{\rm eff}$. P is the projection operator for the model space, and we shall for later use introduce also the corresponding projection operator, Q, for the complementary space, $P+Q=1$. We shall use the *intermediate normalization*, where $\langle\Psi_0^\alpha|\Psi^\alpha\rangle = 1$, $|\Psi_0^\alpha\rangle = P|\Psi^\alpha\rangle$ and $P\Omega P = P$. The effective hamiltonian and the effective perturbation then have the form $H_{\rm eff} = PH\Omega P$ and $H'_{\rm eff} = PH'\,\Omega P$.

Bound-state S-matrix formulation

The standard procedure for treating bound-state QED is based upon the scattering or S-matrix formulation. As a background we shall briefly review this technique for the first-order electron-electron interaction. We consider the case with a single reference state (closed-shell system), which means that the zeroth-order wave functions (ZOF), $\Psi_0 = \Phi$, is known from the start. We add an adiabatic damping factor to the perturbation, $H' \rightarrow H'\,\mathrm{e}^{-\gamma|t|}$, which has the effect that the perturbation is turned on and off smoothly, so that $H \rightarrow H_0$ and $\Psi \rightarrow \Phi$, as $t \rightarrow \pm\infty$.

We work in the *interaction picture*, where the operators and wave functions are related to those in the conventional Schrödinger (or Dirac) picture by

$$O_{\rm I}(t) = \mathrm{e}^{\mathrm{i}H_0 t}\, O_{\rm S}\, \mathrm{e}^{-\mathrm{i}H_0 t}; \qquad \Psi_{\rm I}(t) = \mathrm{e}^{\mathrm{i}H_0 t}\, \Psi_{\rm S}(t).$$

The time-dependent Schrödinger equation then takes the form

$$\mathrm{i}\frac{\partial}{\partial t}\Psi_{\rm I}(t) = H'_{\rm I}\,\Psi_{\rm I}(t) \qquad \Psi_{\rm I}(t) = \Psi_{\rm I}(t_0) - \mathrm{i}\int_{t_0}^{t} \mathrm{d}t'\, H'_{\rm I}(t')\,\Psi_{\rm I}(t'). \tag{5}$$

We introduce the *time-evolution operator*, $U(t,t_0)$, defined by

$$|\Psi_I(t)\rangle = U(t,t_0)|\Psi_I(t_0)\rangle, \tag{6}$$

which has the expansion

$$U(t,t_0) = 1 + \sum_{n=1}^{\infty} \frac{(-\mathrm{i})^n}{n!} \int_{t_0}^{t} \mathrm{d}t_n \ldots \int_{t_0}^{t} \mathrm{d}t_1\, T\big[H'_{\rm I}(t_n)\ldots H'_{\rm I}(t_1)\big] \mathrm{e}^{-\gamma(|t_1|+|t_2|\ldots+|t_n|)}, \tag{7}$$

where T is the Wick *time-ordering operator*. (In the following we shall work only in this picture and leave out the subscript I.)

The interaction between electrons and photons is represented by the perturbation $H' = \psi^\dagger(x) e\alpha^\mu A_\mu \psi(x)$, where A_μ represent the electromagnetic field operators and ψ and $\psi^\dagger$ are the *electron-field operators*, $\psi(x) = \sum_j c_j\,\phi_j(x)$; $\psi^\dagger(x) = \sum_j c_j^\dagger\,\phi_j(x)$. c_j and $c_j^\dagger$ are electron annihilation/creation operators, and $\{\phi_j(x)\}$ is a set of single-electron functions $\phi_j(x) = \phi_j(\boldsymbol{x})\,\mathrm{e}^{-\mathrm{i}\varepsilon_j t}$. ($x$ is the four-dimensional space-time coordinate.) The space parts are solutions to the Dirac equation, $h_D\,\phi_j(\boldsymbol{x}) = \varepsilon_j\,\phi_j(\boldsymbol{x})$ in the field of the nucleus and possibly other electrons. γ is the *adiabatic damping parameter*, which eventually goes to zero, $\gamma \rightarrow +0$. (We employ here *relativistic units*, i.e., $m = c = \epsilon_0 = \hbar = 1$; $\mathrm{e}^2 = 4\pi\alpha$, where α is the fine-structure constant). The scattering or S matrix is defined $S = U(\infty,-\infty)$. The exchange of a single photon between two electrons is represented by the Feynman diagram in Fig. 1 and by the S-matrix element

$$\Big\langle rs\Big|S^{(2)}\Big|ab\Big\rangle = \iint \mathrm{d}^4x_1\mathrm{d}^4x_2\,\phi_r^\dagger(x_1)\phi_s^\dagger(x_2)\,I_{21}\,\phi_b(x_2)\phi_a(x_1), \tag{8}$$

where $I_{21} = -\mathrm{i}e^2\alpha_1^\mu\alpha_2^\nu\,D_{F\nu\mu}(x_2-x_1)$ and $D_{F\nu\mu}(x_2-x_1)$ is the *photon propagator*. Integration over the times leads in the limit $\gamma \rightarrow 0$ to a delta function,

$$\Big\langle rs\Big|S^{(2)}\Big|ab\Big\rangle = 2\pi\,\delta(\varepsilon_r+\varepsilon_s-\varepsilon_a-\varepsilon_b)\,\Big\langle rs\Big|I_{21}(q)\Big|ab\Big\rangle, \tag{9}$$

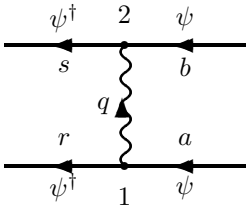

Figure 1: Graphical representation of the S-matrix for single-photon exchange between the electrons. The wavy line represents the photon propagator and the straight lines the electron field.

where $I_{21}(q)$ is the fourier transform of I_{21} and $q = \varepsilon_a - \varepsilon_r = \varepsilon_s - \varepsilon_b$. $V_{21}(q) = \mathrm{i}\, I_{21}(q)$ is an *equivalent interaction* for single-photon exchange, which in the *Feynman gauge* becomes

$$V_{21}^F(q) = \int_0^\infty \frac{2k\,\mathrm{d}k\, f_{21}(k)}{q^2 - k^2 + \mathrm{i}\eta}; \qquad f_{21}(k) = -\frac{e^2}{4\pi^2\, r_{12}}\,(1 - \boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2)\,\sin(kr_{12}) \tag{10}$$

$$\text{or} \qquad V_{21}^F(q) = \frac{e^2}{4\pi\, r_{12}}\,(1 - \boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2)\, e^{\mathrm{i}|q|r_{12}}. \tag{11}$$

The energy shift can be obtained by means of the Gell-Mann–Low–Sucher formula [1, 2], and for the single-photon exchange this leads to $\Delta E = \Big\langle \Phi \Big| V_{21}(q) \Big| \Phi \Big\rangle$.

The delta function in (9) implies that *energy is conserved* during the process – the energy of the final state $(\varepsilon_r + \varepsilon_s)$ is equal to that of the initial state $(\varepsilon_a + \varepsilon_b)$. As mentioned previously, this restricts the applicability of the S-matrix formulation to cases with a single reference function and prevents the use of an extended model space with several reference functions in order to treat quasi-degeneracy in the MBPT way. In the following sections we shall describe a modified procedure, which is free from this limitation.

Time-evolution-operator formalism

The reason for the energy conservation in the S-matrix formulation is the fact that the time integration is extended over the entire time range, from $-\infty$ to $+\infty$. Instead of the S-matrix, we shall investigate the more general *time-evolution operator* $U(t, t_0)$, defined in (6). This is the basic tool in time-dependent perturbation theory, which has been applied in non-QED calculations for a long time [12, 13].

The evolution operator is in standard perturbation theory used only for *forward* time evolution. In order to be able to apply the procedure also to bound-state QED problems, this has to be extended to include *forward as well as backward time evolution*, which will make it possible to adopt the *covariant Feynman approach*. In this way an effective QED hamiltonian of the type (2) can be derived, applicable also to an extended model space.

We consider first systems with a single reference state and as before add an adiabatic damping factor to the perturbation. Gell-Mann and Low [1] have shown that in the limit $\gamma \to 0$

$$|\widetilde{\Psi}\rangle = \frac{|\Psi\rangle}{\langle\Phi|\Psi\rangle} = \lim_{\gamma\to 0} \frac{U(0,-\infty)|\Phi\rangle}{\langle\Phi|(0,-\infty)|\Phi\rangle} \tag{12}$$

is regular and an eigenfunction of the full hamiltonian [14, p. 61], [15, p. 336]. The evolution operator can be represented by diagrams of Goldstone type, which are *linked* as well as *unlinked*. Unlinked diagrams have one or several disconnected, closed parts with the initial as well as the final state in the model (P) space. These diagrams are singular as $\gamma \to 0$ but are eliminated from

the evolution-operator expansion in the ratio (12), which is therefore *regular*. In the intermediate normalization, we then obtain

$$|\widetilde{\Psi}\rangle = \big(1 + Q\,U(0,-\infty)_{\rm Linked}\big)\,|\Phi\rangle, \tag{13}$$

which is the *linked-diagram theorem* [16, 17]. The operator $\big(1+Q\,U(0,-\infty)_{\rm Linked}\big)P$ corresponds to the wave operator in MBPT (3). (P and Q are the projection operators for the model and complementary spaces, respectively.)

The original treatment of Brueckner–Goldstone and Gell-Mann–Low, valid for a single reference state (closed-shell systems), was later generalized to the degenerate case in the 1970's by several groups [13, 18, 19, 20], working mainly with nuclear problems. The Gell-Mann–Low formula (12) can then be generalized to

$$|\widetilde{\Psi}^\alpha\rangle = \lim_{\gamma\to 0}\frac{U(0,-\infty)|\phi^\alpha\rangle}{\langle\phi^\alpha|U(0,-\infty)|\phi^\alpha\rangle}, \tag{14}$$

where $\{\phi^\alpha\}$ are certain functions in the model space. In addition to the unlinked diagrams, singularities may here appear also for linked diagrams with a model-space state appearing as an intermediate state. We refer to such diagrams as *reducible*. The remaining *irreducible* diagrams are *regular*.

In intermediate normalization the zeroth-order wave function, corresponding to (14), is

$$|\widetilde{\Psi}_0^\alpha\rangle = P\,|\widetilde{\Psi}^\alpha\rangle = \lim_{\gamma\to 0}\frac{P\,U(0,-\infty)|\phi^\alpha\rangle}{\langle\phi^\alpha|U(0,-\infty)|\phi^\alpha\rangle}. \tag{15}$$

For convenience we introduce a new operator

$$V(t,-\infty) = U(t,-\infty) - 1, \tag{16}$$

which we rewrite according to

$$V(t,-\infty)\,P = \Big[V(t,-\infty)_{\rm Irr} + \delta V(t,-\infty)\Big]\,P\,U(0,-\infty)\,P. \tag{17}$$

$V(t,-\infty)_{\rm Irr}$ represents the irreducible part of the evolution operator, and the modification operator $\delta V(t,-\infty)$ is defined by this factorization. For the modified operator in the square brackets we introduce a special symbol

$$\widetilde{V}(t,-\infty)_{\rm Irr} = V(t,-\infty)_{\rm Irr} + \delta V(t,-\infty); \qquad V(t,-\infty) = \widetilde{V}_{\rm Irr}(t,-\infty)\,P\,U(0,-\infty)\,P. \tag{18}$$

For *time-independent* interactions, as in nuclear many-body applications, δV can be expressed in terms of *folded* diagrams, which take care of the difference in the time orderings [13]. For *time-dependent* interactions, as in bound-state QED, there will be additional contributions, appearing when the singularities – or the very large contributions in the case of quasi-degeneracy – are eliminated. We refer to these contributions as *Model-Space Contributions, MSC*. [2]

Inserting (17, 18) into the Gell-Mann–Low relation (14), we obtain, using (15),

$$\big|\widetilde{\Psi}^\alpha\big\rangle = \big(1 + Q\,\widetilde{V}(0,-\infty)_{\rm Irr}\big)\,\big|\widetilde{\Psi}_0^\alpha\big\rangle. \tag{19}$$

The operator $\big(1 + Q\,\widetilde{V}(0,-\infty)_{\rm Irr}\big)P$ corresponds to the wave operator in MBPT (3), (13).

From the relation (17) and using $V = U-1$ we obtain (for simplicity leaving out the arguments)

$$\delta V\,PUP = \big(V - V_{\rm Irr}\,PU\big)\,P = \big(V - V_{\rm Irr} - V_{\rm Irr}\,PV\big)\,P$$

[2] These contributions have previously often been referred to as *reference-state contributions*, but since model-space states which are not exactly degenerate (quasi-degenerate) with the intitial (reference) state also contribute, we find that the term model-space contributions more adequate.

$$\text{or} \qquad \delta V = \big(V - V_{\rm Irr} - V_{\rm Irr}\, PV - \delta V\, PV\big)\, P = \big(V - V_{\rm Irr} - \widetilde{V}_{\rm Irr}\, PV\big)\, P.$$

Using (18), this leads to the useful recursive formula

$$\widetilde{V}_{\rm Irr} P = \big(V_{\rm Irr} + \delta V\big)\, P = \big(V - V_{\rm Irr} PV - \delta V PV\big)\, P = \big(V - \widetilde{V}_{\rm Irr} PV\big)\, P$$

and the expansion of the *modified evolution operator*

$$\widetilde{U}_{\rm Irr} P = \big(U - \widetilde{V}_{\rm Irr} P \widetilde{V}_{\rm Irr} - \widetilde{V}_{\rm Irr} P \widetilde{V}_{\rm Irr} P \widetilde{V}_{\rm Irr} - ...\big)\, P, \tag{20}$$

which is our main result in this section. Here, the 'counter terms' eliminate the single, double,... singularities of U – and the corresponding large contributions appearing in the case of quasi-degeneracy. Thus, *the modified evolution operator, $\widetilde{U}_{\rm Irr}$, which is the basic tool in this formalism, is regular in all orders*.

In lowest non-trivial order (20) leads to

$$\widetilde{U}^{(4)}_{\rm Irr}\, P = \big(U^{(4)} - U^{(2)} P U^{(2)}\big)\, P. \tag{21}$$

The contribution to the effective hamiltonian is obtained by the relation [18, 5]

$$H'_{\rm eff} = P \left[\mathrm{i} \frac{\partial}{\partial t} \widetilde{U}(t, -\infty)_{\rm Irr} \right]_{t=0} P. \tag{22}$$

Application of the evolution-operator technique to bound-state QED problems

Single-photon exchange. Covariant form of the evolution operator.

We shall now apply the covariant evolution-operator technique to the interaction between the electrons and start with the single-photon exchange, earlier treated with the S-matrix formalism (Fig. 1). In order to be able to include negative-energy states, it is necessary to allow time to run also in the backward direction, illustrated by the time-ordered (Goldstone) diagrams in Fig. 2. These can be combined into a *Feynman diagram* in Fig. 3 and expressed by the evolution

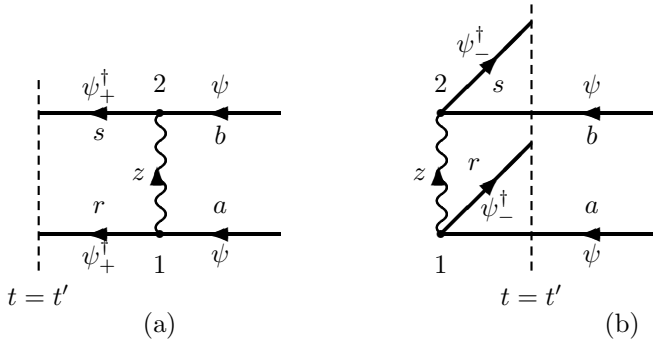

Figure 2: Time-ordered (Goldstone) diagrams representing the evolution operator for single-photon exchange between the electrons for forward (a) and backward (b) time evolution. The subscripts of the field operators indicate particle and hole part, respectively.

operator

$$\langle rs|U^{(2)}_{\rm Cov}(t', -\infty)|ab\rangle = \Big\langle rs \Big| \iint \mathrm{d}t_1\, \mathrm{d}t_2\, \mathrm{i}S_F(x'_1, x_1)\, \mathrm{i}S_F(x'_2, x_2) \times I_{21}\, \mathrm{e}^{it'(\varepsilon_r + \varepsilon_s)}\, \mathrm{e}^{-\mathrm{i}\varepsilon_a t_1 - \mathrm{i}\varepsilon_b t_2}\, \mathrm{e}^{-\gamma(|t_1| + |t_2|)} \Big| ab \Big\rangle. \tag{23}$$

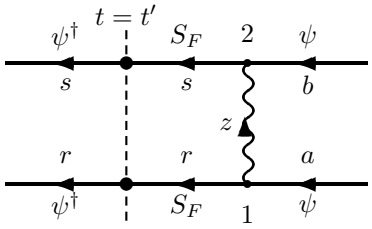

Figure 3: Feynman-type diagram, representating the covariant form of the evolution operator for single-photon exchange. The straight line between dots represents the electron propagator.

Performing the integrations yields

$$\left\langle rs\left|U^{(2)}_{\rm Cov}(t',-\infty)\right|ab\right\rangle = \left\langle rs\left|\int {\rm d}k\, f_{21}(k)\left[\frac{1}{q-(k-{\rm i}\gamma)_r}+\frac{1}{q'-(k-{\rm i}\gamma)_s}\right]\right|ab\right\rangle \times\frac{{\rm e}^{-{\rm i}t'(q+q'+{\rm i}\gamma_r+{\rm i}\gamma_s)}}{q+q'+{\rm i}\gamma_r+{\rm i}\gamma_s} \qquad (q=\varepsilon_a-\varepsilon_r;\ q'=\varepsilon_b-\varepsilon_s;\ \ (A)_x=(A)\,{\rm sgn}(\varepsilon_x)). \tag{24}$$

If the outgoing state $\langle rs|$ lies in the complementary Q space (outside the model space), then $q+q'\neq 0$, and the expression is regular as $\gamma\to 0$. For $t'=0$ this then yields a contribution to the first-order wave operator (3),

$$\Omega^{(1)}=\sum_{|rs\rangle\in Q}\frac{|rs\rangle\langle rs|V_{21}(q,q')|ab\rangle}{\varepsilon_a+\varepsilon_b-\varepsilon_r-\varepsilon_s};\qquad V_{21}(q,q')=\int {\rm d}k\, f_{21}(k)\left[\frac{1}{q-(k-{\rm i}\gamma)_r}+\frac{1}{q'-(k-{\rm i}\gamma)_s}\right]. \tag{25}$$

If the outgoing state $\langle rs|$ lies in the P or model space, we get a contribution to the first-order effective hamiltonian, using (22),

$$\langle rs|H'_{\rm eff}|ab\rangle=\langle rs|V_{21}(q,q')|ab\rangle. \tag{26}$$

The time derivation eliminates here the last denominator in (24), which becomes singular, when $q+q'=0$ – or very large when $q+q'\approx 0$ in the case of quasi-degeneracy. $V(q,q')$ is the *equivalent interaction* to be compared with the S-matrix result (10). It is easy to show that the two results are identical for diagonal elements, but the evolution-operator result is applicable also when energy is not conserved between the initial and final states.

The results (25) and (26) show that in this form of bound-state QED the first-order wave operator and effective hamiltonian are given by expressions quite analogous to those of standard time-independent MBPT [10]. This holds also in higher orders and will open the possibility to combine bound-state QED with MBPT in a systematic fashion [5].

Two-photon electron-electron interaction

We consider next the *two-photon (ladder) exchange*, illustrated in Fig. 4, corresponding to the covariant evolution operator

$$\left\langle rs\left|U^{(4)}_{\rm Cov}(t',-\infty)\right|ab\right\rangle_{\rm Ladder}=\left\langle rs\right|\iint {\rm d}^4x_3\,{\rm d}^4x_4\iint {\rm d}t_1\,{\rm d}t_2\,{\rm i}S_F(x'_4,x_4)\,{\rm i}S_F(x'_3,x_3)\,I_{43} \times{\rm i}S_F(x_4,x_2)\,{\rm i}S_F(x_3,x_1)\,I_{21}\,{\rm e}^{{\rm i}t'(\varepsilon_r+\varepsilon_s)}\,{\rm e}^{-{\rm i}\varepsilon_a t_1-{\rm i}\varepsilon_b t_2}\,{\rm e}^{-\gamma(|t_1|+|t_2|+|t_3|+|t_4|)}\Big|ab\Big\rangle. \tag{27}$$

This can be evaluated in the standard way. The diagram has a *reducible* part, when a model-space state appears as the intermediate state and the two photons do not overlap in time [5].

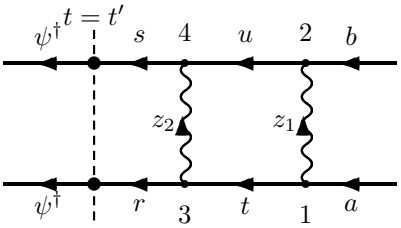

Figure 4: Graphical representation of the covariant evolution operator for the two-photon-photon ladder interaction between the electrons.

The modified operator $\widetilde{U}_{\rm Irr}$ (20, 21), however, is *free from singularities* – as well as from the very large contributions appearing in the case of quasi-degeneracy. No special procedure is needed to evaluate the residual contributions from the reducible diagrams, the so-called *Model-Space Contributions, MSC*. They follow directly from the general expression for $\widetilde{U}_{\rm Irr}$, which is regular. It is easy to show that for elements diagonal in energy the MSC obtained in this way agree with those obtained with the S-matrix formalism, although not necessarily for each diagram separately.

The contribution to the effective hamiltonian is evaluated by means of (22). For elements diagonal in energy the results agree with those obtained with the standard S-matrix formalism [21].

The *crossed two-photon diagram* can be treated in a similar way as the ladder diagram. Here, there is no reducible part, and no counter terms appear.

Application to the fine structure of He-like ions

In earlier works we have reported on second-order QED calculations of the *ground-state energy* of He-like ions, both the *non-radiative* [21] and *radiative* parts [22]. Similar calculations have also been performed by other groups [23, 24]. In the present work we report on corresponding calculations on *excited states* of such ions, restricting ourselves here to the two non-radiative diagrams, the two-photon ladder and the two-photon crossed diagram, discussed above. We have investigated the $1s2p$ multiplet, and for light and medium-heavy elements this requires the use of an *extended model space*, for which the new procedure described here is particular appropriate. Preliminary results with the new technique are here presented for the first time.

Numerical results for 1s2p states

We have employed the same numerical procedure as in our previous calculations [21], but the results are still preliminary. (Our numerical accuracy is presently of the order of 10^{-5} H, and we are presently in the process of improving this at least one order of magnitude.) The calculated energy levels (in LS notations) together with the corresponding experimental values are collected in Table 1. The first two columns give the result in first order – without and with diagonalization of the model-space hamiltonian – the next column the second-order result (with diagonalization), and in the fourth column we have added higher-order many-body effects, obtained in a separate relativistic (non-QED) many-body calculation [4], as well as the mass-polarization, taken from Drake [25]. Finally, comparison is made with the calculations of Drake and with available experimental results [26]. The results are normalized to the state $J = 0$ and given in Hartree atomic units (1H=27.2 eV).

Discussion

The results presented here agree well with the results of Drake [25] as well as with available experimental data [26]. It should be noted, though, that our calculations are still incomplete.

Table 1: *Preliminary results for the 1s2p energy levels of He-like Ne and Ar. The* $^3P_0$ *state is used as reference. Values given in Hartree atomic units (1H=27.2 eV).*

Z	State	First order No diag.	First order Diagonaliz.	Second order Diagonaliz.	Incl. HO MBPT	Drake*	Expt'l**
10	$^1P_1$	0.235	0.3439	0.26103	0.26581	0.26588	
	$^3P_2$	0.0071	0.0071	0.00849	0.00844	0.00846	0.008457(2)
	$^3P_1$	0.1091	0.0007	0.00133	0.00131	0.00136	0.001369(7)
	$^3P_0$	0	0	0	0	0	0
18	$^1P_1$	0.5338	0.6890	0.60979	0.61317	0.61333	
	$^3P_2$	0.1202	0.1202	0.12474	0.12464	0.12481	0.12495(3)
	$^3P_1$	0.1774	0.0223	0.02337	0.02347	0.02360	
	$^3P_0$	0	0	0	0	0	0

* From reference [25] ** From reference [26]

So far, only the *non-radiative QED effects* (two-photon ladder and cross) are included, while the *radiative effects* (vacuum polarization and self energy) remain to be done. (The overall QED effects is for Ne of the order of 50 and for Ar a few hundred μ Hartree.) Furthermore, our calculations are performed in the *Feynman gauge*, and the results are expected to be slightly gauge-dependent. We are presently investigating this dependence.

In the case of the $^3P_2 - ^3P_0$ separation for Ar there is a significant difference between the result of Drake and the new experimental result of Kukla et al [26]. We believe that this is due to higher order many-body-QED effects, and it is our ambition to test this hypothesis by the more complete caclulations that we are now performing.

Summary and conclusions

In this work we have summarized and further developed the bound-state QED formalism, based upon the *covariant form of the time-evolution operator* [5]. With this formalism it is possible to evaluate elements non-diagonal in energy and thereby to apply the extended-model-space procedure, developed in non-QED many-body perturbation theory [10]. This is not possible with the traditional S-matrix formalism, where only elements diagonal in energy can be evaluated. It is demonstrated that the two formalisms lead to the same results for elements diagonal in energy. In the formalism presented here *all singularities are eliminated*. This implies that the evaluation of the *Model-Space Contributions*, i. e., contributions due to model-space states appearing as intermediate states, which is quite cumbersome in the S-matrix formulation and the Gell-Mann–Low–Sucher procedure, is here quite simple. Corresponding contributions appear also for quasi-genenerate model-space states and are evaluated in the same straightforward way.

We have applied the new formalism to an extended model space including the quasi-degenerate states $1s\,2p_{1/2}$ and $1s\,2p_{3/2}$ of some heliumlike ions, and numerical results are presented for the first time. The agreement with available experimental data is quite good. So far, only non-radiative QED effects are included, but calculations of the corresponding radiative effects are under way.

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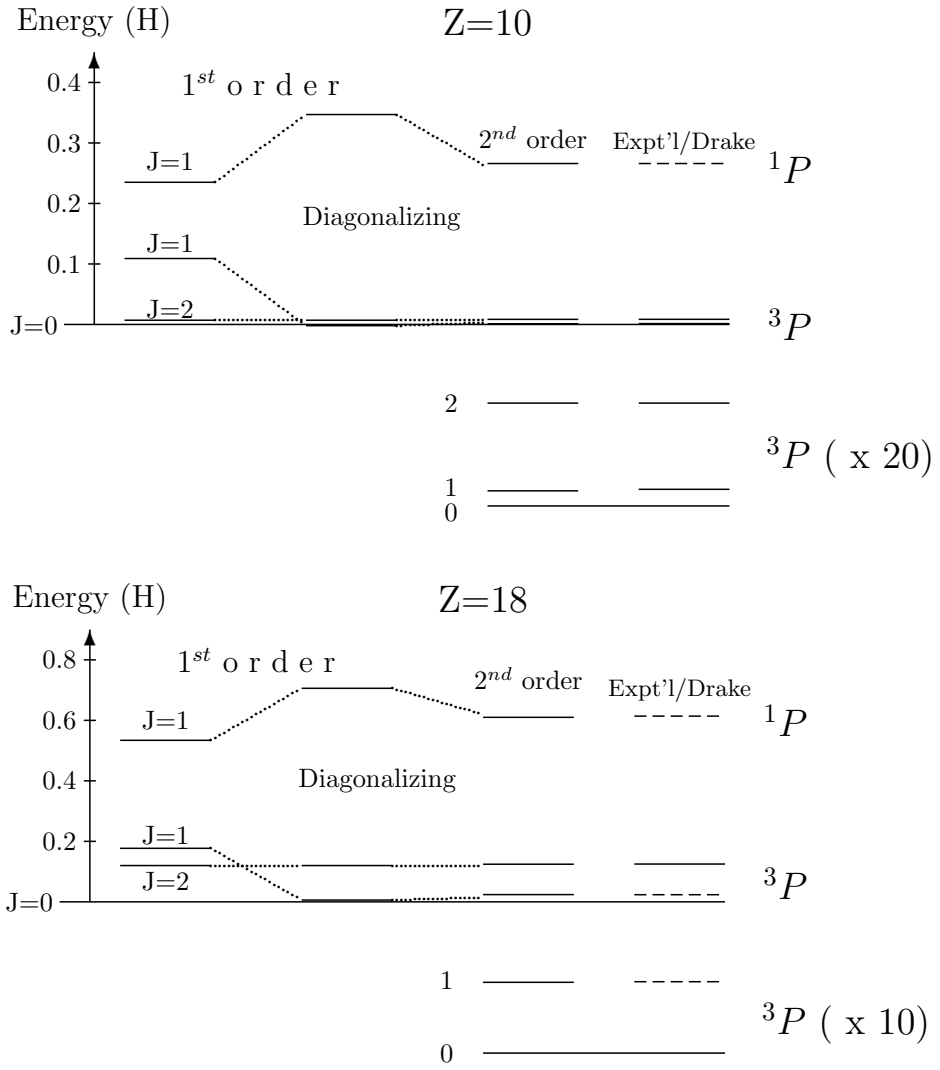

Figure 5: Comparison between the theoretical and experimental energy levels of the $1s\,2p$ multiplet for some He-like ions. Our first-order results are shown in pure j-j coupling as well as after diagonalization of the effective hamiltonian, and the second-order results only after this diagonalization. Comparison is made with experimental results, when available, (full line) and with the theoretical results of Drake [25] (dotted).