

QUASI-DEGENERACY IN BOUND-STATE QED. FINE STRUCTURE OF HELIUMLIKE IONS

INGVAR LINDGREN, STEN SALOMONSON, BJÖRN ÅSÉN, and
ANN-MARIE MÅRTENSSON-PENDRILL

*Department of Physics, Chalmers University of Technology and Göteborg University, SE 41296
Göteborg, Sweden*

A new procedure for bound-state QED, based upon a covariant form of the time-evolution operator is reported. This procedure is applicable also to systems with closely spaced or *quasi-degenerate* levels, where the standard S -matrix formalism can generally not be used due to *quasi-singularities*. We have applied the procedure to the heliumlike ions of neon and argon, and produced the first numerical QED results for a complete fine-structure splitting. Good agreement is obtained with recent experimental data. The new procedure is closely related to standard many-body perturbation theory (MBPT), which may open up possibilities to combine QED and MBPT in a more systematic way.

1 Introduction

There is presently a renewed interest in the study of the fine structure of helium and heliumlike ions, the main reason being that accurate comparison of experimental and theoretical data can lead to an independent determination of the fine-structure constant α ^{1,2,3,4}.

Quite recently a very accurate measurement of the fine-structure separation $2^3P_1 - 2^3P_0$ in neutral helium has been reported with an accuracy of 30 ppb⁵. Compared with accurate analytical calculations⁴ this yields a value of the fine-structure constant, $1/137.0359864(31)$, which *differs from the accepted value by four standard deviations*. Quite accurate values exist also for the separations in heliumlike ions, some of which are shown in Table 1^{6,7,8,9,10,11}.

The most accurate QED calculations on heliumlike ions are performed by means of the analytical $Z\alpha$ expansion, which works well for low Z . For higher Z the convergence rate decreases drastically, and a rapidly increasing number of terms is needed to reach high accuracy. For high Z , where $Z\alpha$ approaches unity, the power expansion cannot be used, and it is necessary to utilize numerical methods, using a Furry-like picture, which corresponds to an expansion to all orders in $Z\alpha$.

The standard numerical technique for bound-state QED is based upon the S -matrix formulation with the Gell-Mann–Low–Sucher procedure^{12,13}. Such calculations have been performed for the ground state of heliumlike ions^{14,15,16,17} and also to some excited states of such ions^{18,19}. Generally, however, this technique is not applicable for excited states with multiplet structure, where the states can be very closely spaced or *quasi-degenerate*. Presently, only two procedures are available for dealing with such problems in its full generality, namely the *two-times Green's-function procedure*, developed by Shabaev and coworkers^{20,21,22,23} and the *covariant evolution-operator procedure*, recently developed by us^{24,25}.

Table 1: Experimental data for some fine-structure separations of He-like ions in the $1s2p$ multiplet. (The values for $Z=2$ and 3 are in MHz, the remaining ones in cm^{-1})

Z	${}^3P_1 - {}^3P_0$	${}^3P_2 - {}^3P_0$	${}^3P_2 - {}^3P_1$	Expt'l method
2	29616.9509(9) ^a		2291.175(1) ^b	Laser spect.
3	155704.3(9) ^c		-62678.4(9) ^c	Laser spect.
7	8.6707(7) ^d			Laser spect.
9			957.8730(12) ^e	Laser spect.
10		1856(1) ^f		Solar flare
12	833,133(15) ^g	4404.6(2,1) ^f		Laser spect./Solar flare
18		27425(5) ^h		Beam foil

^a George *et al.*⁵ ^b Storry *et al.*², Castilla *et al.*³ ^c Riis *et al.*⁶ ^d Thompson *et al.*⁷
^e Myers *et al.*⁸ ^f Curdt *et al.*⁹ ^g Myers *et al.*¹⁰ ^h Kukla *et al.*¹¹

Another approach to deal with the structure of heliumlike ions is to use many-body procedures of various kind, where the electron correlation can be treated essentially to all orders, and corrected for QED effects by using the analytical expansion to leading order. The shortcoming of such an approach is that it is difficult to go beyond the leading order for the QED effects. It would therefore be desirable to be able to combine the MBPT and QED approaches in some systematic way, which seems to be necessary to achieve sufficient accuracy for medium-heavy elements. The present work represents one step in that direction.

The atomic fine-structure is entirely due to relativity and QED, with leading orders of $(Z\alpha)^2$ and $(Z\alpha)^3$, respectively, relative to the non-relativistic energies. For that reason the fine-structure is a good candidate for testing the theory, when very accurate experimental results are becoming available, particularly for heliumlike ions. For high Z a comparison between theory and experiment will test QED at strong electric fields and for low Z this can be used to determine the fine-structure constant, α , provided the theory of QED is trusted.

2 Time-independent perturbation theory. Quasi-Degeneracy

In perturbation theory the Hamiltonian is normally partitioned into a zeroth-order Hamiltonian and a perturbation

$$H = H_0 + H'. \quad (1)$$

Working with a single reference or zeroth-order function, Φ , the standard (Rayleigh-Schrödinger) perturbation theory gives the first-order contribution to the wave function

$$\Psi^{(1)} = \sum_{\Phi^i \neq \Phi} \frac{|\Phi^i\rangle \langle \Phi^i | H' | \Phi \rangle}{E_0 - E_0^i}. \quad (2)$$

The reference function, Φ , also referred to as the *model function*, is in this case an eigenfunction of H_0 and forms together with the remaining eigenfunctions form the basis functions,

$$H_0 \Phi = E_0 \Phi \quad \text{and} \quad H_0 \Phi^i = E_0^i \Phi_i.$$

This can easily be generalized to the case with several *degenerate* reference or model functions, where the summation in (2) runs over states *not* degenerate with the model functions.

In the case of *quasi-degeneracy*, (very closely lying states) some of the energy denominators in (2) can be very small, which may cause serious *convergence problems*. In relativistic many-body perturbation theory (MBPT), applied to the fine structure in the $1s2p$ multiplet of He-like

systems, the states $1s2p_{1/2}$ and $1s2p_{3/2}$ are very close in energy and hence strongly mixed for light elements. This has led to serious problems using a single reference function²⁶, problems which can be remedied by using an *extended model space*^{27,28,29}.

We consider now a number of eigenfunctions of the Hamiltonian

$$H \Psi^\alpha = E^\alpha \Psi^\alpha \quad (\alpha = 1, 2, \dots, d), \quad (3)$$

referred to as the *target functions*. The relation between the target functions and the corresponding *model functions* is given by a *wave operator*,

$$\Psi^\alpha = \Omega \Psi_0^\alpha \quad (\alpha = 1, 2, \dots, d). \quad (4)$$

In the *intermediate normalization* we apply here, the model functions are projections of the corresponding target functions on the model space,

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

The wave operator satisfies the *Bloch equation*^{27,30,28}

$$[\Omega, H_0]P = (H' \Omega - \Omega P H' \Omega)P, \quad (6)$$

Expanding the wave operator order by order, leads instead of (2) to the first-order contribution

$$\Omega^{(1)}|m\rangle = \sum_{i \in Q} \frac{|i\rangle \langle i|H'|m\rangle}{E_0^m - E_0^i}. \quad (7)$$

m/i represents a basis function inside/outside the model space. We see here that there is no (quasi)degeneracy in this expansion.

The Bloch equation can also be used to derive the *linked-diagram expansion* for an extended model space, which can be expressed^{27,28}

$$[\Omega, H_0]P = (H' \Omega - \Omega P H' \Omega)_{\text{Linked}}P \quad (8)$$

In the general case the model functions are not eigenfunctions of H_0 . Instead they are solutions of the secular equation

$$H_{\text{eff}} \Psi_0^\alpha = E^\alpha \Psi_0^\alpha. \quad (9)$$

H_{eff} is matrix operator, acting in the model space and referred to as the *effective Hamiltonian*. The *eigenvectors of the effective Hamiltonian are the model functions* (4) and the *eigenvalues are the corresponding exact energies*. In intermediate normalization the effective Hamiltonian has the form

$$H_{\text{eff}} = PH\Omega P = PH_0P + PH'\Omega P. \quad (10)$$

In the MBPT procedure with an extended model space, the states of the model space are excluded from the summations of the type (7), thus eliminating not only degenerate but also quasi-degenerate states.

The procedure is now to evaluate the matrix elements of the effective Hamiltonian (10), which is diagonalized to yield the exact energies and the model functions. The (quasi)degenerate states are in this procedure mixed to all orders of perturbation theory. If there are states that are completely degenerate in zeroth order with the state considered and of the same symmetry (so that they can mix), then a procedure with an extended model space is more or less mandatory. In the case of quasi-degeneracy the procedure can improve the convergence drastically²⁹.

In the case of the $1s2p$ multiplet of heliumlike ions the two states $(s_{1/2} p_{1/2})_{J=1}$ and $(s_{1/2} p_{3/2})_{J=1}$ have the same symmetry, and for light elements they are closely spaced and hence strongly mixed.

By including these states in the model space their mixture will be appropriately taken care of, which might be quite difficult, using the standard procedure with single reference function.

The main question is now: **Can a similar procedure be applied in bound-state QED?** A major obstacle is here that the standard procedure for bound-state QED, the S -matrix formulation, requires *energy conservation* between the initial and final states and hence cannot be used to evaluate the elements of the effective Hamiltonian (9) *non-diagonal* in energy, needed to treat quasi-degeneracy using an extended model space. Therefore, the procedure has to be modified, as we shall demonstrate below.

3 Time-dependent perturbation theory

In order to find a procedure applicable also to a quasi-degenerate situation, we shall consider *time-dependent perturbation theory*, although the problems we shall study usually are time independent. The basic concept is here the *time-evolution operator*, U , which regulates the development of the wave function in time

$$\Psi(t) \propto U(t, t_0) \Psi(t_0) \quad (t > t_0).$$

We work in the *interaction picture*, where the operators and wave functions are related to those in the conventional Schrödinger picture by ^a

$$O_I(t) = e^{iH_0 t} O_S e^{-iH_0 t}; \quad \Psi_I(t) = e^{iH_0 t} \Psi_S(t).$$

The time-dependent Schrödinger equation takes in this picture the form

$$i \frac{\partial}{\partial t} \Psi_I(t) = H'_I \Psi_I(t),$$

which leads to the expansion ³¹

$$U_\gamma(t, t_0) = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!} \int_{t_0}^t dt_n \int_{t_0}^{t_n} dt_{n-1} \dots \int_{t_0}^{t_2} dt_1 T[H'_I(t_n) H'_I(t_{n-1}) \dots H'_I(t_1)] e^{-\gamma(|t_1|+|t_2|+\dots+|t_n|)}, \quad (11)$$

where T is the time-ordering operator.

Due to the adiabatic damping, the perturbation vanishes in the limits $t \rightarrow \pm\infty$ and the exact wave function becomes equal to the unperturbed function in these limits, $\Phi = \Psi(\pm\infty)$. The wave function in time-independent theory corresponds to the time-dependent function at $t = 0$, $\Psi = \Psi(0)$.

Gell-Mann and Low ¹² have shown that for a single reference function (closed-shell case), Φ , the function

$$\Psi(t) = \lim_{\gamma \rightarrow 0} \frac{U_\gamma(t, -\infty) \Phi}{\langle \Phi | U_\gamma(0, -\infty) | \Phi \rangle}$$

is an eigenfunction of the Hamiltonian (provided the limit exists). The evolution operator has singularities due to *unlinked diagrams*, which are eliminated by the denominator.

When several reference functions are used (multi-dimensional model space), the GML procedure has to be modified ^{32,33},

$$\Psi^\alpha(t) = \lim_{\gamma \rightarrow 0} \frac{U_\gamma(t, -\infty) \phi^\alpha}{\langle \phi^\alpha | U_\gamma(0, -\infty) | \phi^\alpha \rangle}. \quad (12)$$

ϕ^α are here certain 'parent' functions in the model space. In this case the evolution operator has singularities or quasi-singularities also for *linked diagrams*, when a model-space state appears as

^aWe use here relativistic units: $c = m = \hbar = \epsilon_0 = 1$; $e^2 = 4\pi\alpha$.

an intermediate state. This is analogous to the situation in time-independent MBPT, discussed above.

We rewrite now the evolution operator, operating on the model space, as

$$U(t, -\infty) = 1 + \tilde{U}(t, -\infty)PU(0, -\infty), \quad (13)$$

leaving out the subscript γ . This leads to the expansion

$$\begin{aligned} U &= 1 + \tilde{U} + \tilde{U}P\tilde{U} + \tilde{U}P\tilde{U}P\tilde{U} + \dots \\ \tilde{U} &= U - 1 - \tilde{U}P\tilde{U} - \tilde{U}P\tilde{U}P\tilde{U} - \dots \end{aligned} \quad (14)$$

\tilde{U} is referred to as the *reduced evolution operator* and can be shown to be *regular*, i.e., free from (quasi)singularities – the (quasi)singularities are eliminated by the *counterterms* ($-\tilde{U}P\tilde{U}$ etc.) in (14).

For $t = 0$ the definition (13) becomes

$$U(0, -\infty) = 1 + \tilde{U}(0, -\infty)PU(0, -\infty),$$

which leads to

$$U(0, -\infty) = (1 + Q\tilde{U}(0, -\infty))PU(0, -\infty).$$

Inserted in the generalized Gell-Mann–Low relation (12) this becomes

$$\Psi^\alpha = \Psi^\alpha(0) = [1 + Q\tilde{U}(0, -\infty)] \Psi_0^\alpha,$$

where

$$\Psi_0^\alpha = P\Psi^\alpha = \frac{PU(0, -\infty) \phi^\alpha}{\langle \phi^\alpha | U(0, -\infty) | \phi^\alpha \rangle}.$$

This we can compare with the MBPT equation above (4), showing that the *wave operator* becomes

$$\boxed{\Omega = 1 + Q\tilde{U}(0, -\infty)}. \quad (15)$$

The effective interaction is defined

$$H'_{\text{eff}} = H_{\text{eff}} - PH_0P$$

and this can be expressed by means of the reduced evolution operator as^{34,25}

$$\boxed{H'_{\text{eff}} = P \left[i \frac{\partial}{\partial t} \tilde{U}(t, -\infty) \right]_{t=0} P}. \quad (16)$$

4 Bound-state QED

4.1 *S*-matrix

The *S*-matrix is defined

$$S = U(\infty, -\infty), \quad (17)$$

where U is the time-evolution operator above. The *S*-matrix for single-photon exchange between electrons, represented by the Feynman diagram in Fig. 1, is given by

$$S^{(2)} = -\frac{1}{2} \iint d^4x_2 d^4x_1 \hat{\psi}^\dagger(x_1) \hat{\psi}^\dagger(x_2) iI(x_2, x_1) \hat{\psi}(x_2) \hat{\psi}(x_1) e^{-\gamma(|t_1|+|t_2|)}. \quad (18)$$

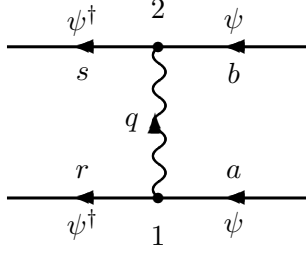


Figure 1: The S-matrix for single-photon exchange

$\hat{\psi}(x)/\hat{\psi}^\dagger(x)$ are the electron-field operators in the *interaction picture*, γ is an *adiabatic-damping factor*, which eventually goes to zero, $\gamma \rightarrow +0$, and

$$I(x_2, x_1) = e^2 \alpha_1^\mu \alpha_2^\nu D_{F\mu\nu}(x_2, x_1), \quad (19)$$

represents the electron-electron interaction, $D_{F\mu\nu}(x_2, x_1)$ being the *photon propagator*. This yields the matrix element^b

$$\begin{aligned} \langle rs | S^{(2)}(x_2, x_1) | ab \rangle &= \\ &= -i \iint dt_1 dt_2 \int \frac{dz}{2\pi} \langle rs | I(z) | ab \rangle e^{-it_1(q-z)} e^{-it_2(q'+z)} e^{-\gamma(|t_1|+|t_2|)}, \end{aligned} \quad (20)$$

where $I(z)$ is the Fourier transform of (19) and $q = \varepsilon_a - \varepsilon_r$; $q' = \varepsilon_b - \varepsilon_s$. After integrations over time and z this becomes

$$\langle rs | S^{(2)} | ab \rangle = -2\pi \Delta_\gamma(q + q') \langle rs | I(q) | ab \rangle,$$

where

$$\int_{-\infty}^{\infty} dt e^{-it(q-z) - \gamma|t|} = \frac{2\gamma}{(q-z)^2 + \gamma^2} = 2\pi \Delta_\gamma(q-z). \quad (21)$$

The relation between the S -matrix and the energy shift is given by the Sucher formula^{13,31}

$$\Delta E = \lim_{\gamma \rightarrow 0} \frac{i\gamma}{2} \frac{\sum_n n \langle rs | S^{(n)} | ab \rangle}{\langle rs | S | ab \rangle}, \quad (22)$$

which in the lowest order ($n = 2$) becomes

$$\Delta E = \lim_{\gamma \rightarrow 0} i\gamma \langle rs | S^{(2)} | ab \rangle. \quad (23)$$

In the present case this gives

$$\Delta E = \delta_{q, -q'} \langle rs | V_{\text{eq}}(q) | ab \rangle. \quad (24)$$

The Kronecker delta factor implies here that the result is nonvanishing only for $q + q' = 0$ or $\varepsilon_a + \varepsilon_b = \varepsilon_r + \varepsilon_s$, which means that energy must be conserved between the initial and final states. This makes the method inapplicable for treating quasi-degeneracy using the method of an extended model space.

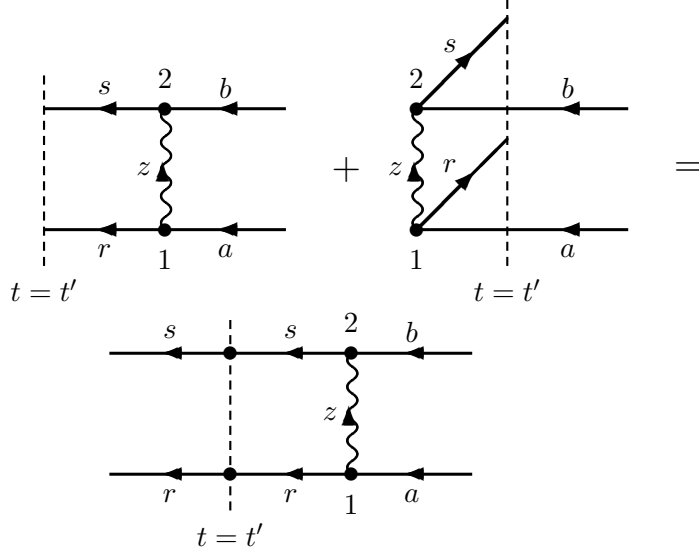


Figure 2: The covariant evolution operator for single-photon exchange.

4.2 Covariant form of the evolution operator

In order to be able to treat the quasi-degeneracy problem, we shall return to the evolution operator, discussed in Sec. 3. However, in dealing with QED problems it is necessary to allow time to run also in the *backward* direction. Therefore, we have to generalize the standard evolution operator as illustrated for single-photon exchange in Fig. 2. This corresponds to the expression^{24,25}

$$U_{\text{Cov}}^{(2)}(t', -\infty) = -\frac{1}{2} \iint d^4x_1 d^4x_2 \left[\Theta(t' - t_1) \hat{\psi}_+^\dagger(x_1) - \Theta(t_1 - t') \hat{\psi}_-^\dagger(x_1) \right] \\ \times \left[\Theta(t' - t_2) \hat{\psi}_+^\dagger(x_2) - \Theta(t_2 - t') \hat{\psi}_-^\dagger(x_2) \right] iI(x_2, x_1) \hat{\psi}(x_2) \hat{\psi}(x_1) e^{-\gamma(|t_1|+|t_2|)}, \quad (25)$$

where Θ is the Heaviside step function. The time integrations are here performed over *all* times, making this operator *covariant* – in contrast to the evolution operator for forward evolution only (11). The operator (25) can also be expressed by means of the *electron propagator* as

$$U_{\text{Cov}}^{(2)}(t', -\infty) = -\frac{1}{2} \iint d^3x'_1 d^3x'_2 \hat{\psi}^\dagger(x'_1) \hat{\psi}^\dagger(x'_2) \times \\ \times \iint d^4x_2 d^4x_1 iS_F(x'_2, x_2) iS_F(x'_1, x_1) iI(x_2, x_1) \hat{\psi}(x_2) \hat{\psi}(x_1) e^{-\gamma(|t_1|+|t_2|)}, \quad (26)$$

which yields the matrix element

$$\langle rs | U_{\text{Cov}}^{(2)}(t', -\infty) | ab \rangle = \\ = \iint dt_1 dt_2 \langle rs | S_F(x'_1, x_1) S_F(x'_2, x_2) iI(x_2, x_1) | ab \rangle e^{it'(\varepsilon_r + \varepsilon_s)} e^{-it_1\varepsilon_a - it_2\varepsilon_b} e^{-\gamma(|t_1|+|t_2|)}. \quad (27)$$

^bWe use here the *Furry picture*, where the single-electron orbitals are solutions of the Dirac equation in the field of the nucleus (and possibly other electrons), $V(r)$,

$$h_D \phi_i = [\mathbf{p} \cdot \boldsymbol{\alpha} + \beta + V(r)] \phi_i = \varepsilon_i \phi_i.$$

We use the Dirac notations $|ab\rangle$ for straight products (not antisymmetrized) of single-particle functions, and the matrix-element notation $\langle || \rangle$ includes integration over the *space* coordinates.

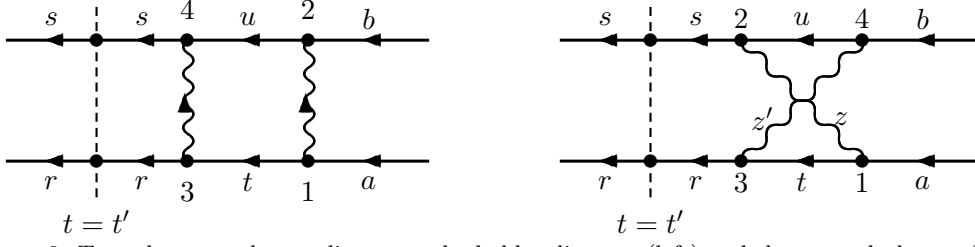


Figure 3: Two-photon exchange diagrams, the ladder diagram (left) and the crossed-photon diagram (right).

After time integrations this becomes

$$\langle rs | U_{\text{Cov}}^{(2)}(t', -\infty) | ab \rangle = \langle rs | V(q, q') | ab \rangle \frac{e^{-it'(q+q'+i\gamma_r+i\gamma_s)}}{q+q'+i\gamma_r+i\gamma_s}, \quad (28)$$

where γ_x has the same sign as ε_x . Using the Feynman gauge we obtain

$$V(q, q') = \int dk f(k) \left[\frac{1}{q - (k - i\gamma)_r} + \frac{1}{q' - (k - i\gamma)_s} \right], \quad (29)$$

where $q = \varepsilon_a - \varepsilon_r$; $q' = \varepsilon_b - \varepsilon_s$ and

$$f(k) = -\frac{e^2}{4\pi^2 r_{12}} (1 - \boldsymbol{\alpha}_1 \cdot \boldsymbol{\alpha}_2) \sin(kr_{12}).$$

The contributions to the first-order wave operator (15) and effective interaction (16) then become

$$\Omega^{(1)} = Q U_{\text{Cov}}^{(2)}(0, -\infty) = \sum \frac{|rs\rangle \langle rs | V(q, q') | ab \rangle}{\varepsilon_a + \varepsilon_b - \varepsilon_r - \varepsilon_s} \quad (30)$$

$$\langle rs | H_{\text{eff}}^{(1)} | ab \rangle = \langle rs | \left[i \frac{\partial}{\partial t} U_{\text{Cov}}^{(2)}(t, -\infty) \right]_{t=0} | ab \rangle = \langle rs | V(q, q') | ab \rangle. \quad (31)$$

In the first case the state $|rs\rangle$ lies in the complementary space (outside the model space) and in the second case inside the model space. The effective interaction agrees with the S -matrix result, when initial and final energies are the same. But the important point is here that the evolution-operator result is valid also when these energies are different, making the procedure applicable also to an extended model space with several unperturbed energies.

Another important advantage of the evolution-operator method is that – in contrast to the S -matrix formulation (22) – no limiting procedure of the adiabatic damping factor γ is needed. (This factor is here used only to indicate the position of possible poles.) This implies that the integrations can be performed independently with *exact energy conservation* at each vertex. This simplifies considerably the treatment of (quasi)singularities, as we shall demonstrate with the two-photon exchange below.

4.3 Two-photon exchange

There are two Feynman diagrams, representing the two-photon exchange between the electrons, the 'ladder diagram' and the 'crossed-photon diagram', illustrated in Fig. 3. The covariant evolution operator for the ladder diagram is given by

$$\langle rs | U_{\text{Cov}}^{(4)}(t', -\infty) | ab \rangle = \langle rs | \iint d^4x_3 d^4x_4 iS_F(x'_3, x_3) iS_F(x'_4, x_4) iI(x_4, x_3) \times \\ \times \iint dt_1 dt_2 iS_F(x_3, x_1) iS_F(x_4, x_2) iI(x_2, x_1) | ab \rangle e^{it'(\varepsilon_r + \varepsilon_s)} e^{-it_1\varepsilon_a - it_2\varepsilon_b} e^{-\gamma(|t_1| + |t_2| + |t_3| + |t_4|)}, \quad (32)$$

and similarly for the crossed diagram.

The ladder diagram has a (quasi)singularity, when the intermediate state (tu) is (quasi)-degenerate with the initial state (ab). In order to study this (quasi)singularity, we first separate the ladder into a *separable* and a *non-separable* part. A diagram is said to be separable, if *the two photons do not overlap in time*, or in other words that there exists an intermediate time ($t = t''$), for which there is no free photon, as indicated in the leftmost diagram in Fig. 4. *If the intermediate state of a separable diagram lies in the model space, the diagram is said to be reducible.*

It can be shown that the separable two-photon diagram is given by²⁵

$$\langle rs | U_{\text{Sep}}^{(4)}(t', -\infty) | ab \rangle = \langle rs | V(q + p', q' + p) | tu \rangle \langle tu | V(p, p') | ab \rangle \frac{e^{-it'(q+q')}}{(q + q')(p + p')}, \quad (33)$$

where $q = \varepsilon_a - \varepsilon_r$; $q' = \varepsilon_b - \varepsilon_s$ and $p = \varepsilon_a - \varepsilon_t$; $p' = \varepsilon_b - \varepsilon_u$. The corresponding contribution to the effective Hamiltonian is then, using (16),

$$\frac{\langle rs | V(q + p', q' + p) | tu \rangle \langle tu | V(p, p') | ab \rangle}{p + p'}, \quad (34)$$

which is (quasi)singular, when the intermediate state (tu) is (quasi)degenerate with the initial state (ab) ($p + p' \approx 0$).

In the expression for the effective interaction (16), the *reduced* evolution operator (11) appears. In the present case this operator is given by

$$\tilde{U}^{(4)} = U^{(4)} - U^{(2)} P U^{(2)}, \quad (35)$$

and the *counterterm*, $-U^{(2)} P U^{(2)}$, is here

$$\frac{\langle rs | V(q - p, q' - p') | tu \rangle \langle tu | V(p, p') | ab \rangle}{p + p'}. \quad (36)$$

If we introduce $W(E_0) = V(q + p', q' + p) = V(E_0 - \varepsilon_r - \varepsilon_u, E_0 - \varepsilon_s - \varepsilon_t)$ with $\Delta E = p + p' = E_0 - \varepsilon_t - \varepsilon_u$, the contribution to the effective Hamiltonian can be expressed

$$\frac{\langle rs | W(E_0) - W(E_0 - \Delta E) | tu \rangle}{\Delta E} \langle tu | V(p, p') | ab \rangle. \quad (37)$$

This expression is *regular* – free from (quasi)singularities. When $\Delta E \rightarrow 0$ (complete degeneracy), the result becomes

$$\left\langle rs \left| \left[\frac{\delta}{\delta E} W(E) \right]_{E=E_0} \right| tu \right\rangle \langle tu | V(p, p') | ab \rangle, \quad (38)$$

which is identical to the S -matrix result. The result (37), however, is more general and (as the single-photon result) valid for a model space that is not necessarily degenerate. A similar result can be derived for the wave operator, which is also regular.

When a separable two-photon diagram is *irreducible* (not reducible), then there is no counterterm, and the contribution to the effective Hamiltonian is given by (34). The summation is then performed only over intermediate states in the *complementary space* (Q), and there is no (quasi)degeneracy. This is then quite similar to the standard expression of second-order perturbation theory (2), which is entirely contained in the separable two-photon diagram. In addition, the separable two-photon diagram contains QED effects – beyond standard MBPT – due to negative energy states and retardation.

The remaining, non-separable part of the ladder diagram is always regular, and this is also the case of the crossed two-photon diagram, which has no reducible part. These parts can be

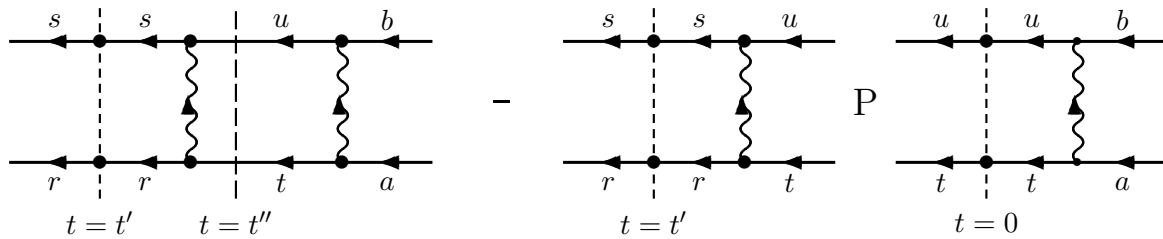


Figure 4: The reduced evolution operator for the two-photon exchange. The second diagram represents the counterterm $U^{(2)}PU^{(2)}$ in (35)

evaluated in a straightforward manner. The non-separable diagrams represent pure QED effects – with no analogy in MBPT.

The above illustrates the close analogy between standard MBPT and bound-state QED using the covariant-evolution-operator method – a fact which may open up possibilities of combining QED and MBPT in a more systematic fashion than has previously been possible.

5 Results and discussion

We have applied the covariant-evolution-operator method to evaluate the fine-structure separation of the $1s2p$ multiplet of the He-like ions of Ne and Ar, and the results are reproduced in Table 2. Our calculations include the exchange of one and two photons between the electrons, as described above, which contains relativistic many-body effects to second order in addition to the QED effects. Furthermore, we have included relativistic electron correlation effects *beyond* second order from a separate many-body calculation. The remaining QED effects, not included in the diagrams evaluated, namely the self-energy and vacuum-polarization contributions, are estimated by means of the analytical $Z\alpha$ expansion. Our numerical results are compared with those of Drake³⁵ and Plante *et al.*²⁶, as well as with available experimental results^{11,9}.

Our calculation represents the first application of bound-state QED to a quasi-degenerate fine-structure separation, using a numerical technique to *all orders* of $Z\alpha$. The results of our calculations agree very well with available experimental data.

Our results agree also well with those of Drake and Plante *et al.* The calculations of Drake are performed using highly correlated non-relativistic wave functions of Hylleraas type with relativistic and QED effects estimated from the analytical expansion. In the work of Plante *et al.* a relativistic MBPT procedure is used, with the QED correction separately added.

For the elements presented here the difference between the theoretical results is hardly significant compared to the experimental and theoretical uncertainties. (For the argon ion the result of Drake differs from the experimental result by 2-3 standard deviations, which is likely due to inaccuracy in the relativistic correction.) When higher accuracy is needed, however, higher-order QED effects will be important. Already for argon we have found that the effects beyond the leading $(Z\alpha)^3$ order are at least comparable to that of the leading term.

As can be seen from Table 1, quite accurate experimental data are available for neutral helium as well as for the ions of lithium and fluorine. For very low Z the numerical problems increase, due to slow convergence of the partial-wave expansion. In addition, the electron correlation plays here a relatively more important role, and two-photon exchange may not be sufficient. For these reasons, it will be difficult at present to compete with the analytical results for He and Li^+ . In order to achieve higher accuracy with the numerical technique, it would be necessary to combine the QED and MBPT procedures in some way, and developments along these lines

Table 2: Comparison between experiment and theory for the fine-structure separations the $1s2p$ multiplet of some He-like ions (in μ Hartree $\approx 27,2 \mu$ eV).

Z	${}^3P_1 - {}^3P_0$	${}^3P_2 - {}^3P_0$	${}^3P_2 - {}^3P_1$	
10	1371(7) 1361(6) 1370 1373	8458(2) 8455(6) 8469 8464		Expt'l ⁹ Drake ³⁵ Plante <i>et al.</i> ²⁶ Present ²⁵
18	23600(60) 23690 23792	124960(30) 124810(60) 124942 124938		Expt'l ¹¹ Drake ³⁵ Plante <i>et al.</i> ²⁶ Present ²⁵

are in progress. A good test of the present procedure described here, however, would be to try to reproduce the experimental result of the fluorine ion, which has an accuracy of the order of one ppm. Here high-order QED effects will certainly be significant. Such an accurate numerical result could then be used to test the analytical expansion and possible to estimate higher-order non-calculated terms. In this way the numerical results could contribute to the accuracy of the theoretical result also for very low Z and possibly to the evaluation of the fine-structure constant.

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