QED procedure applied to the quasidegenerate fine-structure levels of He-like ions

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A procedure for bound-state QED is presented, based upon a covariant form of the time-evolution operator. In contrast to the standard *S*-matrix formalism, our procedure is applicable also to states that are *quasidegenerate*. All (quasi)singularities, which appear when an intermediate state is (quasi)degenerate with the initial state, are eliminated. Our procedure is closely related to many-body perturbation theory (MBPT) and may open up possibilities to combine QED and MBPT in a more systematic fashion. The procedure is applied to the fine structure of the heliumlike neon and argon ions, and good agreement is obtained with recent experimental data.

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I. INTRODUCTION

There is presently great interest in the study of the fine structure of helium and heliumlike ions, one reason being that accurate comparison of experimental and theoretical data can lead to an independent determination of the fine-structure constant α [1–4].

The experimental situation regarding heliumlike ions up to 1995 has been reviewed by Kukla *et al.* [5]. More recently, measurements have been performed using an electron-beam ion trap [6,7] and by studying solar flares [8]. Of particular interest are the extremely accurate results of Myers *et al.*, using Doppler-tuned fast-beam laser spectroscopy [9–11].

Calculations on heliumlike ions have been performed particularly by Drake [12], using highly correlated nonrelativistic wave functions, corrected for relativity and QED by means of analytical results for the leading terms of the $Z\alpha$ expansion. Relativistic many-body calculations have been performed mainly by the Notre Dame group [13,14] and to a lesser extent by our group [15]. Relativistic multiconfiguration Dirac Fock (MCDF) calculations have been performed by the Oxford and Paris groups [16,17].

Numerical QED calculations to all orders in $Z\alpha$ for the ground state of heliumlike ions have been performed by us and other groups [18–21]. Corresponding calculations on excited states [22] have been hampered by the fact that the standard technique for bound-state QED calculations, the *S*-matrix formulation with the Gell-Mann–Low–Sucher procedure [23,24], is not applicable to systems with *quasidegeneracy*, i.e., systems with very closely spaced energy levels. The only procedures available to such problems, known to us, are the *two-times Green's-function procedure*, developed by Shabaev and co-workers [25–28], and the *covariant evolution-operator procedure*, recently developed by us [29,30]. We present here numerical all-order results for the quasidegenerate fine-structure levels of some He-like ions, using our technique. (Preliminary results from this work were presented at the workshop *QED2000* in Trieste, Italy, October 2000 [30].)

In the $1s2p$ multiplet of He-like systems, there are two states with $J=1$, in the j-j scheme represented by $1s2p_{1/2}$ and $1s2p_{3/2}$, respectively. For light and medium-heavy elements these states are very closely spaced and strongly mixed. Systems of this kind are best treated by means of the *extended-model-space procedure*, for a long time applied in atomic many-body theory [15,31,32]. In this scheme, a *wave operator*, Ω, and an *effective Hamiltonian*, $H_{\rm eff}$, are set up for a model space containing the quasidegenerate states in question. The wave operator generates the corresponding exact wave functions, or *target states*, when operating on the zeroth-order functions or *model states*,

$$\Psi^{\alpha}=\Omega\,\Psi_0^{\alpha}, \tag{1.1}$$

and the effective Hamiltonian, operating entirely within the model space, reproduces the corresponding *exact energies* of the target states,

$$H_{\rm eff}\Psi_0^{\alpha}=E^{\alpha}\Psi_0^{\alpha}. \tag{1.2}$$

The model states are eigenstates of the effective Hamiltonian. In the *intermediate normalization*, which we employ here, the model functions are projections on the model space of the full wave functions,

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

and the effective Hamiltonian has the form

$$H_{\rm eff}=PH\Omega P. \tag{1.4}$$

In order to set up an effective Hamiltonian for a multidimensional, quasidegenerate model space, it is necessary to evaluate also *elements nondiagonal in energy*. This is the crucial point, which makes the standard *S*-matrix formulation inapplicable. We shall demonstrate here that this can be remedied by means of the covariant evolution-operator technique, leading to a procedure quite analogous to that used in many-body perturbation theory (MBPT). We shall illustrate this by means of the $1s2p$ multiplet of the He-like neon and argon ions.

II. TIME-DEPENDENT MBPT

We partition the Hamiltonian into a (time-independent) zeroth-order Hamiltonian, H_0, and a perturbation, $H'(t)$,

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which might be time-dependent,

$$H = H_0 + H'(t). \tag{2.1}$$

In the *interaction picture* (I) the operators and wave functions are related to those in the conventional Schrödinger (or Dirac) picture (S) by

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

The time-dependent Schrödinger equation then takes the form

$$i\frac{\partial}{\partial t}\Psi_I(t) = H'_I(t)\Psi_I(t). \tag{2.2}$$

The (forward) time evolution of the wave functions is given by the standard *time-evolution operator*, $U(t,t_0)$,

$$\Psi_I^\alpha(t) = U(t,t_0)\,\Psi_I^\alpha(t_0), \tag{2.3}$$

which satisfies the equation

$$i\frac{\partial}{\partial t}U(t,t_0) = H'_I(t)U(t,t_0) \tag{2.4}$$

and has the expansion

$$U(t,t_0) = 1 + \sum_{n=1}^{\infty} \frac{(-i)^n}{n!}\int_{t_0}^{t} dt_n \cdots \times \int_{t_0}^{t} dt_1 T[H'_I(t_n)\cdots H'_I(t_1)] e^{-\gamma(|t_1|+|t_2|\cdots+|t_n|)}. \tag{2.5}$$

Here, T is the Wick *time-ordering operator* and γ is the *adiabatic damping parameter*, which eventually goes to zero, $\gamma \to +0$. (In the following we shall work entirely in the interaction picture and leave out the subscript I.)

The full functions of time-independent MBPT (1.1) correspond to the time-dependent functions at $t=0$ and the zeroth-order wave function (1.3) to the limit $t \to -\infty$,

$$\Psi^\alpha = \Psi^\alpha(t=0), \qquad \Psi_0^\alpha = \Psi^\alpha(t \to -\infty). \tag{2.6}$$

According to a generalization of the original Gell-Mann–Low formula [23] to a multidimensional model space [33,34], the target functions can be expressed

$$\Psi^\alpha(t) = \lim_{\gamma\to 0} \frac{U(t,-\infty)\,\phi^\alpha}{\langle \phi^\alpha | U(0,-\infty) | \phi^\alpha \rangle}, \tag{2.7}$$

where $\{\phi^\alpha\}$ are certain "*parent*" functions lying in the model space. In addition to the singular, unlinked diagrams, appearing in the nondegenerate case, singularities may for a degenerate model-space state appear also for linked diagrams, when a degenerate state appears as an intermediate state. In the case of a *quasidegenerate* model space, also *quasisingularities* may appear, i.e., finite but very large contributions, when quasidegenerate states appear as intermediate states. All diagrams with intermediate model-space states are referred to as *reducible*. The remaining *irreducible* diagrams are *regular* with no (quasi)degeneracies.

All singularities as well as quasisingularities are eliminated in Eq. (2.7), but when the interaction is time- or energy-dependent, as in QED, there will in general also be a *residual finite contribution*, which we refer to as the *model-space contribution* (MSC).

In order to derive an expression for the MSC, we introduce a new operator $\tilde{U}$—which we refer to as the *reduced evolution operator*—by means of the relation

$$U(t,-\infty)P = P + \tilde{U}(t,-\infty)PU(0,-\infty)P. \tag{2.8}$$

The new operator, $\tilde{U}$, is *regular*, and all singularities and quasisingularities of U are contained in the factor $PU(0,-\infty)P$. $\tilde{U}$ contains the irreducible part of U as well as the MSC. This relation can be regarded as a generalization of the factorization theorem for time-independent perturbations, used particularly in nuclear theory [33,34].

For $t=0$ we have from Eq. 2.8

$$U(0,-\infty)P = PU(0,-\infty)P + QU(0,-\infty)P = [1 + Q\tilde{U}(0,-\infty]PU(0,-\infty)P, \tag{2.9}$$

where $Q = 1-P$ is the projection operator for the complementary space (outside the model space). The generalized Gell-Mann–Low relation (2.7) for $t=0$ then yields

$$\Psi^\alpha = \Psi^\alpha(0) = \lim_{\gamma\to 0}[1 + Q\tilde{U}(0,-\infty)] \frac{PU(0,-\infty)\phi^\alpha}{\langle \phi^\alpha | U(0,-\infty) | \phi^\alpha \rangle}. \tag{2.10}$$

Using the intermediate normalization (1.3), the model functions are

$$\Psi_0^\alpha = P\,\Psi^\alpha = \lim_{\gamma\to 0} \frac{PU(0,-\infty)\,\phi^\alpha}{\langle \phi^\alpha | U(0,-\infty) | \phi^\alpha \rangle}, \tag{2.11}$$

and the target functions (2.10) can be expressed

$$\Psi^\alpha = [1 + Q\tilde{U}(0,-\infty)]\Psi_0^\alpha. \tag{2.12}$$

The operator $[1+Q\tilde{U}(0,-\infty)]$ corresponds to the wave operator (1.1) in time-independent MBPT. We can then express the effective Hamiltonian in intermediate normalization (1.4) as

$$H_{\rm eff} = PH[1 + Q\tilde{U}(0,-\infty)]P. \tag{2.13}$$

We define the *effective interaction*, $H'_{\rm eff}$, by

$$H_{\rm eff} = PH_0P + H'_{\rm eff} \tag{2.14}$$

or

$$H'_{\rm eff} = PH'\Omega P = PH'[1 + Q\tilde{U}(0,-\infty)]P. \tag{2.15}$$

Using Eq. (2.8) together with Eq. (2.4), we obtain

$$i\left[\frac{\partial}{\partial t}U(t,-\infty)\right]_{t=0}P=i\left[\frac{\partial}{\partial t}\tilde{U}(t,-\infty)\right]_{t=0}PU(0,-\infty)P$$
$$=H'\,U(0,-\infty)P$$

and with the factorization theorem (2.9)

$$i\left[\frac{\partial}{\partial t}U(t,-\infty)\right]_{t=0}P=H'[1+Q\tilde{U}(0,-\infty)]PU(0,-\infty)P.$$

This leads with Eq. (2.15) to the useful form of the effective interaction

$$H'_{\rm eff}=P\left[i\frac{\partial}{\partial t}\tilde{U}(t,-\infty)\right]_{t=0}P. \tag{2.16}$$

We note that in this form of the effective interaction it is the *closed* part of $\tilde{U}$ that contributes.

The definition (2.8) of the reduced evolution operator leads directly to the expansion

$$UP=P+\tilde{U}P+\tilde{U}P\tilde{U}P+\tilde{U}P\tilde{U}P\tilde{U}P+\cdots \tag{2.17}$$

for simplicity leaving out the arguments [which are $(t,-\infty)$ for the first, open operator and $(0,-\infty)$ for the closed operators between the P operators]. The expansion for the reduced evolution operator then becomes

$$\tilde{U}P=UP-P-\tilde{U}P\tilde{U}P-\tilde{U}P\tilde{U}P\tilde{U}P-\cdots. \tag{2.18}$$

The terms $\tilde{U}P\tilde{U}P,\tilde{U}P\tilde{U}P\tilde{U}P$, etc. are (quasi)singular and can be shown to eliminate all single, double, . . . singularities and quasisingularities of the original evolution operator, U. We refer to these terms as "*counterterms*." In the lowest nontrivial order, Eq. (2.18) yields

$$\tilde{U}^{(4)}P=(U^{(4)}-U^{(2)}PU^{(2)})P, \tag{2.19}$$

and below we shall apply that to the two-photon exchange between electrons and demonstrate that it is regular.

III. APPLICATION TO QED

In the standard evolution operator (2.3), time runs only in the *forward* direction, but in order to be able to apply this operator to QED problems, we shall allow time to run also in the *backward* direction, making the operator *covariant*. This is illustrated in Fig. 1 for the single-photon exchange between electrons. Using the Feynman gauge, the matrix element of the covariant evolution operator becomes [29,30]

$$\langle rs|U^{(2)}_{\rm cov}(t',-\infty)|ab\rangle$$
$$=\langle rs|V(q,q')|ab\rangle\frac{e^{-it'(q+q'+i\gamma_r+i\gamma_s)}}{q+q'+i\gamma_r+i\gamma_s}$$

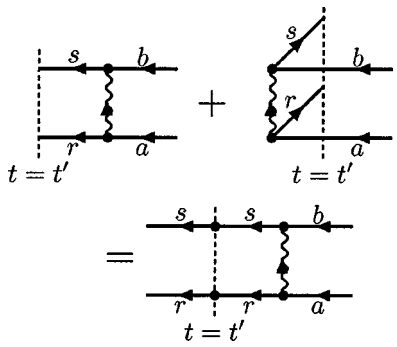

FIG. 1. The evolution operator for single-photon exchange between the electrons including forward and backward time evolution, represented by two time-ordered (Goldstone) diagrams (top) and a single Feynman diagram (bottom). The wavy lines represent the photon propagator and the straight lines between dots the electron propagator.

$$V(q,q')=\int dk\, f_{21}(k)\left[\frac{1}{q-(k-i\gamma)_r}+\frac{1}{q'-(k-i\gamma)_s}\right],$$

$$f_{21}(k)=-\frac{e^2}{4\pi^2 r_{12}}(1-\alpha_1\alpha_2)\sin(kr_{12}),$$

where $(A)_x=(A)\,\mathrm{sgn}(\varepsilon_x)$ and $q=\varepsilon_a-\varepsilon_r;q'=\varepsilon_b-\varepsilon_s$. As usual for this type of calculation, the Furry picture is used [18–22], which means that the orbitals are solutions of the Dirac equation in the field of the nucleus, $V(r)$,

$$h_D|i\rangle=[m\,\mathbf{p}\cdot\boldsymbol{\alpha}+\beta mc^2+V(r)]\,|i\rangle=\varepsilon_i|i\rangle. \tag{3.1}$$

If the outgoing state $\langle rs|$ lies in the complementary Q space, the expression is regular and yields for $t'=0$ a contribution to the first-order wave operator,

$$\Omega^{(1)}=\sum_{|rs\rangle\in Q}\frac{|rs\rangle\langle rs|V(q,q')|ab\rangle}{\varepsilon_a+\varepsilon_b-\varepsilon_r-\varepsilon_s}. \tag{3.2}$$

If the outgoing state $\langle rs|$ lies in the model space, we get a contribution to the first-order effective Hamiltonian (1.4),

$$\langle rs|H'_{\rm eff}|ab\rangle=\langle rs|V(q,q')|ab\rangle. \tag{3.3}$$

The result (3.3) is consistent with the result of the two-times Green's function [25] and reduces to the well-known S-matrix result, when the initial and final states have the same energy $(q+q'=0)$. The result (3.2) has no analog in the other procedures.

For the *two-photon exchange* between the electrons, the covariant evolution operator can be set up in analogy with the single-photon case [29,30]. For a diagram where the two photons do not overlap in time, we introduce the term *separable*—to be distinguished from a *reducible* diagram, which is separable with the intermediate state in the model space (see Fig. 2, top). For a general separable second-order ladder diagram, the contribution to the effective Hamiltonian (1.4) is [29]

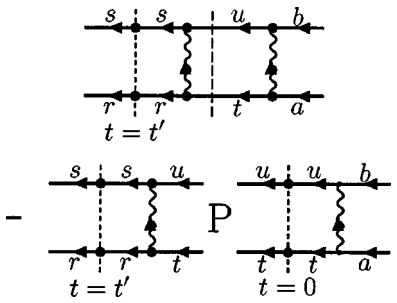

FIG. 2. Graphical representation of the reducible two-photon-photon ladder diagram and the corresponding counter term (2.19).

$$\frac{\langle rs|V(q+p',q'+p)|tu\rangle\langle tu|V(p,p')|ab\rangle}{p+p'}, \quad (3.4)$$

where $p=\varepsilon_a-\varepsilon_t, p'=\varepsilon_b-\varepsilon_u$. When the diagram is reducible, there is a counterterm (2.19), represented by the second diagram in Fig. 2 and given by

$$-\frac{\langle rs|V(q-p,q'-p')|tu\rangle\langle tu|V(p,p')|ab\rangle}{p+p'}. \quad (3.5)$$

Introducing

$$W(E_0)=V(q+p',q'+p)=V(E_0-\varepsilon_r-\varepsilon_u,E_0-\varepsilon_s-\varepsilon_t),$$

which for given r,s,t,u is a function of $E_0=\varepsilon_a+\varepsilon_b$, the sum of the ladder and the counterterm can be expressed as

$$\frac{\langle rs|W(E_0)-W(E_0-\Delta E)|tu\rangle}{\Delta E}\langle tu|V(p,p')|ab\rangle \quad (3.6)$$

with ΔE being (the negative of) the excitation energy of the intermediate model-space state, $\Delta E=p+p'=E_0-\varepsilon_t-\varepsilon_u$. This shows that the counterterm cancels the (quasi)singularity of the reducible ladder diagram. In the limit of complete degeneracy ($\Delta E\to 0$), the first factor of (3.6) approaches the derivative of the interaction with respect to the energy, which is consistent with the *S*-matrix result. The result (3.6), however, is exactly valid also in the case of quasidegeneracy, or for a nondegenerate model space in general. A similar expression can be derived for the MSC of the wave operator. Also here, the counterterm (2.19) eliminates the (quasi)singularity.

The expression (3.4) is summed over all intermediate states in the Q space and is quite analogous to the second-order expression in standard (time-independent) perturbation theory, which is completely contained in (3.4). This illustrates the close analogy with standard MBPT, a fact which will open up the possibility of combining QED and MBPT in a more systematic fasion than has previously been possible.

The remaining, nonseparable part of the ladder diagram and the entire crossed two-photon diagram, which is also nonseparable, are both regular and can be evaluated in a straightforward manner.

IV. NUMERICAL RESULTS

The procedure presented here is applied to the $1s2p$ states of the He-like ions of Ne and Ar, and the results are given in Table I. We have employed the same numerical procedure as in our previous calculations [19], and the accuracy is at least 10^{-5} hartrees. The third and fourth columns show our first- and second-order QED result, obtained after diagonalizing the effective Hamiltonian with one and two photons, respectively. In the next column, we have added the higher-order many-body effects, obtained in a separate relativistic (non-QED) many-body calculation [15], as well as the mass polarization, taken from Drake [12]. In the following column we have estimated from analytical work [12,35,36] the QED effects, not included in our numerical work. Finally, comparison is made with the calculations of Drake and of Plante *et al.* [14] as well as with available experimental results [5,8].

V. DISCUSSION

The results of our calculation agree very well with available experimental data, as well as with the more approximate

TABLE I. The $1s2p$ energy levels of He-like Ne and Ar. The $^3P_0$ state is used as a reference. Values given in hartree atomic units (1 hartree$=2hc\,\mathcal{R}=27.2$ eV, where $\mathcal{R}$ is the Rydberg constant, corrected for the Bohr mass shift).

Z	State	QED		High. ord.	Remain.	Total	Plante	Drake[c]	Experimental[d]
		one photon	two photon	MBPT	QED	theory	*et al.*		
10	$^1P_1-{}^3P_0$	0.343 88	−0.082 83	0.004 79	0.000 04	0.265 88	0.265 86	0.265 88	
	$^3P_2-{}^3P_0$	0.007 12	0.001 37	−0.000 05	0.000 02	0.008 46	0.008 47	0.008 46	0.008 458(2)
	$^3P_1-{}^3P_0$	0.000 67	0.000 72	−0.000 02	0.000 00	0.001 37	0.001 37	0.001 36	0.001 371(7)
18	$^1P_1-{}^3P_0$	0.689 00	−0.079 00	0.003 39	0.000 40	0.613 80	0.613 46	0.613 33	
	$^3P_2-{}^3P_0$	0.120 18	0.004 56	−0.000 09	0.000 29	0.124 94	0.124 94	0.124 81	0.124 96(3)
	$^3P_1-{}^3P_0$	0.022 32	0.001 33	0.000 10	0.000 04	0.023 79	0.023 69	0.023 60	

[a]From Refs. [12,35,36].
[b]From Ref. [14].
[c]From Ref. [12].
[d]From Refs. [5,8].

QED calculations of Plante *et al*. and of Drake. The present calculation differs from the previous calculations in several important aspects. The calculation of Drake is an accurate nonrelativistic many-body calculation but the relativistic and QED effects are included only to the leading order in $Z\alpha$ by means of analytical expressions. The calculation of Plante *et al*. is an all-order relativistic MBPT calculation with a single-reference model space, including the QED effects of Drake. In the present work, we have evaluated for a quasidegenerate system the relativistic *and* the QED effects numerically to *all* orders of $Z\alpha$. The higher-order QED effects in the present cases are not large enough compared to the experimental and numerical accuracy to exhibit significant differences in the various calculations. These effects will be important, however, when higher acccuracy is needed or in application to heavier ions.

It should be noted that only the *nonradiative* QED corrections (two-photon ladder and cross) have been calculated numerically in our present work. The remaining *radiative* two-electron effects (screened self energy and vacuum polarization) have been included using analytical leading-order results. We have found that for the nonradiative part, effects beyond the leading $(Z\alpha)^3$ order are at least comparable to and for Ar even dominating over the leading term. Therefore, in order to perform a calculation of high accuracy, it is of vital importance to evaluate all the QED effects to all orders in $Z\alpha$. Work along these lines is now in progress.

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