Convergence of relativistic perturbation theory for the $1s2p$ states in low-Z heliumlike systems

A.-M. Mårtensson-Pendrill, I. Lindgren, E. Lindroth, S. Salomonson, and D. S. Staudte
Department of Physics, Chalmers University of Technology, S-412 96 Göteborg, Sweden
and Göteborg University, S-412 96 Göteborg, Sweden
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In a recent paper, Plante *et al.* [Phys. Rev. A **49**, 3519 (1994)] presented relativistic all-order many-body calculations for $n = 1$ and $n = 2$ states of heliumlike ions with nuclear charge in the range Z =3–100. They were, however, unable to obtain converged solutions for the $^1P_1$ states for low Z ($Z \leq 6$). We demonstrate in the present work how application of the "extended model space formulation" by Lindgren [J. Phys. B **7**, 2441 (1974)] leads to convergence also for these cases.

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I. INTRODUCTION

Recent experimental developments have raised the demands for accurate calculations including relativistic as well as quantum electrodynamic (QED) effects. Although much of the methods developed for nonrelativistic many-body calculations can be taken over, the relativistic generalization encounters problems of both practical and formal character. The electron-electron interaction is no longer simply the Coulomb interaction between the electrons. Magnetic interactions lead to the Breit interaction and also retardation effects must eventually be considered. Further, unless contributions from crossed photons are included, the energies obtained depend on the choice of gauge [1–4]. The existence of negative energy solutions to the one-electron Dirac equation requires special treatment. As a first approximation, they are excluded (the "no-virtual-pair" approach), by surrounding the electron-electron interaction with projection operators onto positive energy states. This is now routinely handled by excluding the negative energy states from the summation over the basis functions [5–7]. Methods, based on QED, are now being developed to go beyond the no-virtual-pair approach and include retardation and radiative effects [8–12].

The demands on computer time and storage increase in the relativistic treatment since the quantum numbers nl of a nonrelativistic orbital are replaced by nlj, where $j = |l \pm 1/2|$. In addition, each relativistic orbital is associated with two radial functions, whereas one function suffices in the nonrelativistic case. However, this problem is less serious due to the development of computers.

The formal problem we consider in this work may be of a more unexpected character: In the nonrelativistic limit the orbital energy does not depend on the total angular momentum j, but only on n and l. For the two-electron case, the nonrelativistic configuration $1s2p$, e.g., leads in the relativistic case to a linear combination of the $1s2p_{1/2}$ and $1s2p_{3/2}$ configurations, with slightly different energy. Both configurations enter for the $2\,^1P_1$ and $2\,^3P_1$ states. The mixing between these two configurations cannot be expected to be well described by a perturbation expansion starting from only one of them. Plante *et al.* [13] attempt to circumvent this problem by using as a starting point for the $J = 1$ states a superposition of these two congurations obtained by diagonalizing the Hamiltonian between the two unperturbed configurations. Nevertheless, they were unable to obtain convergence for the $2\,^1P_1$ state for low Z (≤ 6).

A general formalism, capable of dealing with quasidegenerate as well as degenerate and nondegenerate model spaces, was developed two decades ago by Lindgren [14] with a view to problems like the $1s^22s^2$ ground state of beryllium, which has a very large admixture of the $1s^22p^2$ configuration. The Be problem has, indeed, been studied by several groups using extended model spaces [15–21] and the formalism is used extensively in quantum chemistry. The use of an extended model space sometimes, like in the case of Be, leads to problems with intruder states and various approaches have been devised in attempts to circumvent the resulting convergence problems [17,20,21]. We have, however, not encountered intruder problems in the calculations presented here.

All-order methods based on the formalism by Lindgren have been used for a long time in our group within the "coupled-cluster approach" [22]. Our first applications used a numerical solution of the resulting two-dimensional radial equation in a nonrelativistic framework [15,23–26], and attempts were also made to generalize this approach to the relativistic case [27,28]. Later work in our group has instead relied on a numerical basis set obtained by diagonalizing a discretized one-electron Hamiltonian, relativistically as well as nonrelativistically [7,29]. Recent applications have included ground and excited states of heliumlike [7,29–32], lithiumlike [33–35], and berylliumlike [36–38] systems, as well as large-scale calculations for heavier alkalilike systems [39,40,34] and other atoms with one valence electron [41–43]. The calculations for the $2s2p$ states in Be-like systems by Lindroth and Hvarfner [38] are completely analogous to the calculation for the $1s2p$ states in He-like systems, except for the added complication of a $1s^2$ core to deal with in the four-electron case.

Generalized Rayleigh-Schrödinger perturbation theory

We summarize here briefly the general Rayleigh-Schrödinger perturbation formalism by Lindgren [14]. The starting point is the choice of a model Hamiltonian H_0 and a suitable model space, spanned by d eigenstates Φ_0^i to H_0:

$$H_0\Phi_0^i = E_0^i\Phi_0^i. \tag{1}$$

There is considerable freedom in choosing the model space, and it is advantageous to include strongly mixing configurations. In the case of the $1s2p$ states of He-like systems, a natural choice includes the two $1s2p$ configurations, coupled to $J = 1$:

$$\begin{aligned}\Phi_0^1 &= \left\{\left|1s2p_{1/2}\right\rangle_{J=1}\right\},\\ \Phi_0^2 &= \left\{\left|1s2p_{3/2}\right\rangle_{J=1}\right\}.\end{aligned} \tag{2}$$

The projection onto the model space is denoted by

$$P = \sum_i^d \left|\Phi_0^i\right\rangle\left\langle\Phi_0^i\right|.$$

and $Q = 1 - P$ gives the projection onto the orthogonal space, spanned by all other configurations. Here, d is the dimension of the model space, and there are normally d well-defined eigenstates Ψ^a of the full Hamiltonian, which have their major part within the model space and satisfy the equation

$$H\Psi^a = (H_0 + V)\,\Psi^a = E_0^i\Psi^a. \tag{3}$$

In *intermediate normalization*, the "model functions" Ψ_0^a are given by the projections of the eigenstates, Ψ^a, onto the model space, i.e.,

$$\Psi_0^a = P\Psi^a \qquad (a = 1, 2, ..., d).$$

If the model functions are linearly independent, there is a one-to-one correspondence between the d exact solutions and the model functions. It is then possible to define a single *wave operator* Ω which transforms all the model states back to the corresponding exact states,

$$\Psi^a = \Omega\Psi_0^a \qquad (a = 1, 2, ..., d).$$

The existence of a single energy-independent wave operator is in contrast, e.g., to the Brillouin-Wigner form of perturbation theory, where the wave operator is energy dependent, and we note that also the calculation by Plante *et al.* [13] uses energy-dependent expressions. The wave operator satisfies a generalized Bloch equation [44,14]

$$[\Omega, H_0] = V\Omega - \Omega PV\Omega. \tag{4}$$

By acting on Eq. (3) with P, we find the effective Hamiltonian H_{eff} which generates the exact eigenvalues when operating on the model functions:

$$H_{\text{eff}} = PH\Omega P = PH_0\Omega P + PV\Omega P. \tag{5}$$

The model functions are obtained by diagonalization of H_{eff} within the model space. For low Z a diagonalization of the electrostatic interaction, $1/r_{12}$, in the model space spanned by the functions in Eq. (2) leads, to a very good approximation, to the singlet and triplet states

$$\begin{aligned}\Psi_0^1 &\approx (1s2p)^1\,P_1 = \sqrt{\frac{1}{3}}\Phi_0^1 + \sqrt{\frac{2}{3}}\Phi_0^2,\\ \Psi_0^2 &\approx (1s2p)^3\,P_1 = \sqrt{\frac{2}{3}}\Phi_0^1 - \sqrt{\frac{1}{3}}\Phi_0^2.\end{aligned} \tag{6}$$

For low Z, these coefficients are good approximations also after inclusion of correlation effects. Even for $Z = 10$, the weight of the dominating configuration in the model function is only 69%.

II. THE $1s2p$ STATES IN HELIUMLIKE SYSTEMS

The generalized Bloch equation (4), together with the expression (5) for the effective Hamiltonian, and the model space spanned by the states in (2) provide the necessary formalism to treat the $1s2p$ states in heliumlike systems. We present here results for a few low-Z systems, where the convergence is slower than for higher Z. The relativistic pair program based on a numerical basis set developed by Salomonson and Öster [7,36] was used in the calculations.

Since we base our calculation on the Bloch equation (4), including both the $1s2p$ configurations in the model space, the small energy difference between them never leads to small energy denominators — all mixing between them is treated by diagonalizing the 2×2 matrix of H_{eff} in Eq. (5) between the $J = 1$ states.

There are several ways of rearranging terms in Eq. (4), corresponding to resummation of various series of terms [45,46], which may affect the convergence, for better or for worse. Plante *et al.* [13] have shifted part of the energy correction term $\Omega PV\Omega$ to the left-hand side. They then solve for one state at a time: after the initial diagonalization which gives a first approximation to the model functions Ψ_0^a and first-order energies $E_a^{(1)}$, each state is treated separately. Wave-function corrections within the model space are accounted for by a perturbative treatment of off-diagonal elements of the Hamiltonian matrix betwen these states:

$$\tilde{\Psi}_0^{a(n)} = \Psi_0^a + \frac{\Psi_0^b\left\langle\Psi_0^b\right|\,V\Omega^{(n-1)}\left|\tilde{\Psi}_0^{a(n-1)}\right\rangle}{E_a^{(n-1)} - E_b^{(1)}}. \tag{7}$$

The matrix element in Eq. (7) accounts for correlation contributions to the singlet-triplet mixing. It vanishes in the nonrelativistic limit and is, of course, very small for low Z. However, the denominator can also be very small. For example, in the case of $Z = 2$, the converged singlet energy is very close to the first-order triplet energy. The resulting small energy denominator in Eq. (7) is an artifact arising from a nonsymmetric treatment of the two states. For higher Z, the problem is less pronounced, since the energy difference between the $2p_{1/2}$ and $2p_{3/2}$ orbitals is larger. To illustrate this problem, we show in Table I the first-order energies obtained after diagonaliza-

TABLE I. Contributions to the ionization energies of the $2\,^1P_1$ and $2\,^3P_1$ states of heliumlike systems (hartree atomic units).

Contribution \ Z	2	3	4	5	6	10
		$2\,^1P_1$				
First (rel) [a]	0.019 749 29	-0.345 380 80	-0.960 556 97	-1.825 840 41	-2.941 315 26	-9.907 573 76
Corr. (C) [b]	-0.143 593 9	-0.147 989	-0.150 306	-0.151 720	-0.152 679	-0.154 720
Total (C) [c]						
This work	-0.123 844 7	-0.493 370	-1.110 863	-1.977 561	-3.093 994	-10.062 293
RCI [d]			-1.110 857 4		-3.093 987 6	-10.062 286
RMBPT [e]						-10.062 304
Total (DCB) [f]						
This work	-0.123 845 6	-0.493 377	-1.110 884	-1.977 606	-3.094 079	-10.062 692
RCI [d]			-1.110 878 6		-3.094 073 3	-10.062 691
RMBPT [e]						-10.062 710
Drake [g]	-0.123 845 22	-0.493 376 69	-1.110 883 48	-1.977 607 65	-3.094 081 22	-10.062 695 1
		$2\,^3P_1$				
First (rel) [a]	-0.048 527 55	-0.447 800 87	-1.097 149 13	-1.996 669 74	-3.146 497 32	-10.252 922 86
Corr. (C) [b]	-0.084 637 7	-0.079 940 4	-0.077 958 8	-0.076 894 2	-0.076 248	-0.075 278
Total (C) [c]						
This work	-0.133 165 2	-0.527 741 3	-1.175 108 0	-2.073 563 9	-3.222 746	-10.328 201
RCI [d]			-1.175 107 8	-2.073 563 8	-3.222 745 4	-10.328 201
RMBPT [e]						-10.328 202
Total (DCB) [f]						
This work	-0.133 162 7	-0.527 722 4	-1.175 048 2	-2.073 428 2	-3.222 489	-10.326 815
RCI[d,h]			-1.175 048 3	-2.073 428 6	-3.222 489 2	-10.326 817
RMBPT [e]		-0.527 722 9	-1.175 048 6	-2.073 429 2	-3.222 489 9	-10.326 815
Drake [g]	-0.133 162 76	-0.527 722 02	-1.175 048 47	-2.073 428 65	-3.222 489 2	-10.326 815 3

[a]First-order results including the $2p$ eigenvalue and the first-order energy contribution due to the Coulomb interaction.
[b]Correlation energies due to the Coulomb interaction.
[c]Total energy in the Dirac-Coulomb approach.
[d]Cheng *et al.* [48].
[e]Plante *et al.* [13].
[f]Total ionization energy in the Dirac-Coulomb-Breit approximation. Quadratic effects in the Breit interaction are omitted. The final results tabulated in Refs. [13,48] include QED and mass polarization corrections. These terms were subtracted, giving the DCB values in this table.
[g]Drake [50]. As discussed in the text, certain corrections of order $(\alpha)^3$ have been added to the sum $J_{\mathrm{nrel}} + J_{\mathrm{rel}} + J_{\mathrm{ns}}$.
[h]Chen *et al.* [49] ($Z = 5$).

tion of the Hamiltonian $H = H_0 + V$ within the model space spanned by the $1s2p$ configurations. The corresponding nonrelativistic ionization energies are given by

$$E_1(^{1,3}P) = (-Z^2/8 + 59Z/243) \pm (112Z/6561). \quad (8)$$

Analysis of the convergence pattern shows that for $Z \leq 4$ higher orders in the Coulomb interaction are sufficient to bring the singlet energy below the first-order triplet energy. For these Z values, the triplet state thus acts as an "intruder," and it is easily seen that this situation can lead to an energy denominator in Eq. (7) very close to zero. Also for $Z = 5, 6$ the final singlet energy is sufficiently close to the first-order triplet energy to explain the convergence problems encountered by Plante *et al.* for these states.

Convergence

Even when both $J = 1$ states are treated together in the model space, the convergence is very slow. About 70 iterations were needed to obtain the results shown in Table I for $Z = 2$. We emphasize that this slow convergence is *not* related to the near degeneracy of the two $1s2p$ states in the relativistic formulation, but is present also in analogous nonrelativistic calculations for these states [47,30]. It can be ascribed to hydrogenic orbitals giving a somewhat unstisfactory starting point, in particular for the excited orbitals, which feel the unscreened nuclear potential and their full interaction with the $1s$ electron must be treated by sp pair excitations in perturbation theory.

One possibility to improve the convergence is to use excited orbitals generated in a potential which includes at least the dominating part of the interaction with the $1s$ electron, while the $1s$ orbital still sees only the unscreened nuclear potential, e.g.,

$$V_{\rm proj} = (1 - |1s\rangle\langle 1s|) \left\langle 1s \left| \frac{1}{r_{12}} \right| 1s \right\rangle (1 - |1s\rangle\langle 1s|), \quad (9)$$

where the projection $(1 - |1s\rangle\langle 1s|)$ excludes any effect on the $1s$ states by this correction term and still ensures a Hermitian potential. This approach was tested in nonrelativistic applications, where it was found to give significantly improved convergence, in particular for the first few iterations. As a test we performed iterations including only excitations to sp configurations. Just after three iterations, the result based on the potential in Eq. (9) was comparable to that obtained after 30 iterations starting from the hydrogenic orbitals. Also the continued iterations converge better; the result after 20 iterations converged to about seven decimal places, compared to about 70 iterations needed for hydrogenic orbitals. The converged result is independent of the starting point (apart from differences in the no-virtual-pair approach, arising from the potential-dependent definition of negative energy states, which give negligible contributions for low Z).

III. RESULTS

Table I shows the separate contributions to the ionization energies obtained for the $(1s2p)J = 1$ states in the Dirac-Coulomb-Breit (DCB) approximation. For the low-Z values studied here, the first-order result is very close to the corresponding nonrelativistic value, Eq. (8), where the singlet-triplet splitting is proportional to Z. The Coulomb correlation contributions vary relatively little for the Z values in the table, and we recall that in the nonrelativistic limit, the second-order contribution is independent of the nuclear charge, whereas the contributions in nth order decrease as Z^{n-2}. Our total ionization energies within the Dirac-Coulomb no-virtual-pair approach are compared to corresponding results, where available, obtained by Cheng *et al.* [48] and by Chen *et al.* [49] using a relativistic configuration-interaction (RCI) approach and by Plante *et al.* [13] using relativistic many-body perturbation theory (RMBPT).

The effect of the Breit interaction was obtained as the difference between the Dirac-Coulomb and results obtained when the Breit interaction was included to lowest order in the pair equation [37]. For the calculations for these low-Z values, we did not include contributions due to two or more orders in the Breit interaction. For $Z = 10$ these were found to contribute only 4 μhartree for the $2\,^3P_1$ state and 0 μhartree for the $2\,^1P_1$ states [13].

Our Breit contributions, as well as the total Dirac-Coulomb-Breit results are compared to those obtained in Refs. [49,48,13]. The DCB results can also be compared to the values, $J_{\rm nrel} + J_{\rm rel} + J_{\rm ns}$, given by Drake in his extensive tabulation [50]. (The nuclear size correction $J_{\rm ns}$ is automatically included in the numerical calculations using a finite nuclear charge distribution.) However, calculations in the "no-virtual-pair approximation" used here include also certain effects of order $(\alpha)^3$ (a.u.) [51,3,52] which are part of the QED correction $J_{\rm QED}$ tabulated by Drake [50]. The contribution due to the Coulomb interaction alone is $(\alpha)^3\,(-\pi/2 - 5/3)\,\langle\delta(\mathbf{r}_{12})\rangle$, with a much larger effect due to the combination of the Coulomb and Breit interactions: $(\alpha)^3\,(2\pi + 4)\,\langle\delta(\mathbf{r}_{12})\rangle$ [51,12]. Following Drake, we use the values for $\langle\delta(\mathbf{r}_{12})\rangle$, obtained by Accad *et al.* [53]. The corrections obtained in this way are included in the values by Drake shown in Table I. For $Z = 10$, they amount to 4.29 μhartree. [The correction $(19/3 - \pi/2)\,(2/243\pi)\,(Z\alpha)^3$ given in earlier work [11,48,13] also includes the correction due to second order in the Breit interaction, which was not included in our calculations. It also uses the lowest-order approximation $\langle\delta(\mathbf{r}_{12})\rangle \approx (2/243\pi)\,Z^3$, which is not valid for low-Z values.]

Uncertainties in our calculated values arise from the grid extrapolation — our calculations were performed in three logarithmic grids, with 81, 101, and 121 points in the range $e^{-7.6}/Z$ to $e^{4.4}/Z$ and extrapolation was used to remove errors of order $O(h^4)$ and $O(h^5)$. The remaining error due to the finite step size, h, is believed to be less than 0.1 μhartree and is negligible compared to the uncertainty due to contributions from higher angular momenta. Our calculation included orbital angular

momenta up to $l = 10$. To account for higher l values, we studied the behavior in a sequence as higher and higher l values were included. For the Coulomb interaction, the decrease of the contributions is essentially described by l^{-4} and l^{-6}, respectively, for the singlet and triplet states, whereas the Breit contributions (and also relativistic corrections to the Coulomb correlation) converge much slower, as l^{-2} and l^{-4}, respectively. We note that for the l^{-2} (l^{-4}) convergence, the tail amounts to about 9.5 (2.8) times the contribution due to $l = 10$ orbitals. A problem in going to higher and higher l values is that the cusp at $r_1 = r_2$ in the expression $r_<^k/r_>^{k+1}$ in the multipole expansion makes the contributions from higher angular momenta very sensitive to grid effects. In second order, the contributions from higher l values are very similar for the different systems; in the nonrelativistic limit, they are, in fact, independent of Z. However, higher-order effects reduce the tail contributions to the Dirac-Coulomb energy from its second-order value of about 24 μhartree for the $2\ ^1P_1$ to 1.4 μhartree for $Z = 2$ and to about 16(2) μhartree for $Z = 10$. The angular extrapolation, in fact, dominates the final uncertainty and is a problem shared also by the relativistic CI approach and by other methods based on expansion in one-electron basis sets. The angular extrapolation is even more critical for the Breit interaction, with its slower angular convergence. For low Z, the whole Breit interaction is so small that this does not pose a problem, whereas for $Z = 10$, an estimated contribution of 5(2) μ hartree from higher angular momenta is included in the value for the singlet state.

We have shown that the coupled-cluster approach with the technique of extended model space can give accurate results for the $(1s2p)J = 1$ states also for low Z. More detailed applications to systems of experimental interest will be published elsewhere.

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