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Coupled continuum perturbative Feshbach approach to calculate total and partial widths: ${}^{1,3}S^e(3lnl)$ resonant states of He, C^{4+}, N^{5+}, and O^{6+}

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We apply a perturbative method, which takes into account the interaction between different open channels, to calculate total and partial widths of atomic resonances in the framework of the Feshbach formalism. The method requires the calculation of elastic, e.g., noncoupled open-channel wave functions, as in the case in which only one channel is open, thus avoiding the solution of complicated systems of coupled differential equations. As an illustration we have calculated energy positions, total and partial widths of ${}^{1,3}S^e(3lnl)$ resonant states of He, C^{4+}, N^{5+}, and O^{6+}. Our results show that the accuracy reached with this simple approach is comparable to other different non-Feshbach methods and that neglect of the coupling between different open channels can be considered as a reasonable approximation to obtain total and partial widths.

I. INTRODUCTION

Resonant states of atomic systems have received increasing attention from the theoretical point of view in the past few years.[1-17] The simplest atomic resonances are those of doubly excited states of $I^{(Z-2)+}$ heliumlike heavy ions whose energy positions lie in a single continuum of the $I^{(Z-1)+}$ ion. These are populated in collisions of the type

$$I^{Z+} + \mathrm{He} \rightarrow I^{**(Z-2)+} + \mathrm{He}^{2+} \rightarrow I^{(Z-1)+} + \mathrm{He}^{2+} + e^{-}$$

for $Z<5$. When $Z \geq 5$, more than one continuum channel is open, and the $I^{(Z-1)+}$ ion eventually produced after the electron emission can be in an excited state. In this case, the existence of several ionization thresholds considerably complicates the treatment, specially in the calculation of resonance widths. Besides, most authors do not calculate the contributions of the different continua to the width, while knowledge of these partial widths is very useful when the corresponding branching ratios are indispensible to interpret double capture experiments.[18,19] Furthermore, in recent years some experimental groups have begun to measure partial widths of resonant states of He-like ions.[20,21] In some cases, they have used some theoretical inputs to interpret their experiments and their results are still far from being definite.

The Feshbach theory[22] of autoionizing resonances has furnished the theoretical background of a great number of atomic calculations for doubly excited states above one single ionization threshold. When more than one ionization limit is involved, applications are scarce, mainly due to the computationally involved implementation of the method. Very recently, Martín *et al.*[11,12] have proposed an easier way to calculate closed-channel functions by making use of a parallelism between the Feshbach-O'Malley theory for the treatment of doubly excited states,[22,23] and the Phillips-Kleinman nonlocal pseudopotential.[24] This method has been shown to be very useful, especially when more than one ionization threshold is open, and to provide energy positions that are in fairly good agreement with experimental results and the theoretical data obtained with other more ellaborate approaches.[25]

On the other hand, in the Feshbach method one should solve a complicated system of coupled differential equations for each open channel in order to obtain the corresponding partial widths. The sum of such partial widths easily provides the total width of the resonant state considered. In practice, one usually uncouples these open-channel equations by neglecting the interaction between different channels.[2,11,13,25-27] The resulting continuum functions are then the solutions of the problem in a zero-order approximation (they are exact solutions in the limit $Z=\infty$). In the case of large nuclear charges ($Z=5-10$), screened Coulomb functions may be used to represent the continuum. Therefore, it seems reasonable to use the static exchange approximation (which goes beyond the Coulomb approximation) to represent the continuum in the case of a large-Z charge. This approximation has provided total widths that are in good agreement with results obtained with other different methods.[25] However, in spite of this approximation being largely used before, the corrections due to the coupling between different continua has never been quantitatively evaluated.

The aim of this paper is to test the "uncoupled" approximation by explicit inclusion of the interaction between the different open channels and to provide a simple method to improve it without completely destroying this simple "uncoupled" picture (Sec. II). As benchmark systems to apply our method, we have chosen the $^{1,3}S^e(3lnl)$ resonant states of He, C^{4+}, N^{5+}, and O^{6+} (Sec. III). Atomic units are used throughout unless for total and partial widths which are given in electron volts (eV).

II. THEORY

We consider the problem of two electrons moving in the field of a charge Z. We have to solve the Schrödinger equation

$$(\mathcal{H}-E)\Psi=0 \ , \tag{1}$$

where $\mathcal{H}$ is the nonrelativistic Hamiltonian of the system. In the Feshbach formalism,[22] the resonant wave function Ψ is written as a sum of a closed-channel $Q\Psi$ and open-channel $P\Psi$ components

$$\Psi=P\Psi+Q\Psi \ , \tag{2}$$

where P is a projection operator such that asymptotically $P\Psi=\Psi$, and $Q=1-P$. For a two-electron system the P operator has the form[23,28,29]

$$P=P_1+P_2-P_1P_2 \ , \tag{3}$$

where P_i is a one-electron projection operator given by

$$P_i=\sum_{\alpha=1}^{N_t} P_i^{\alpha}=\sum_{\alpha=1}^{N_t} |\phi_\alpha(\mathbf{r}_i)\rangle\langle\phi_\alpha(\mathbf{r}_i)| \tag{4}$$

for a series of autoionizing states converging to the N_t+1 threshold, ϕ_α is the hydrogenic function for the electron i, and α represents the set of quantum numbers (nlm).

A. Closed-channel wave function

In the standard Feshbach method,[22] the closed-channel wave function $\Phi_n^{LS\pi}$ is the eigensolution of the projected equation

$$(Q\mathcal{H}Q-E_n^r)Q\Phi_n^{LS\pi}=0 \ , \tag{5}$$

where E_n^r is the unshifted energy of the resonant state, L and S are the total angular momentum and the total spin, respectively, and π is the parity. When E_n^r is over more than one ionization threshold [$N_t>1$ in Eq. (4)], the solution of Eq. (5) is extremely expensive if a basis set of nonhydrogenic orbitals is used. Instead, we use the pseudopotential Feshbach method of Martín *et al.*[11,12] which replaces Eq. (5) by

$$(\mathcal{H}+V_{\rm PS}-E_n^{\rm PS})\,{}^{\rm PS}\Phi_n^{LS\pi}=0 \ , \tag{6}$$

where $V_{\rm PS}$ is a pseudopotential defined by

$$V_{\rm PS}=MP \tag{7}$$

and M is a large, but otherwise arbitrary, positive number. It has been shown[11,12] that both standard and pseudopotential Feshbach methods are mathematically equivalent since

$${}^{\rm PS}\Phi_n^{LS\pi} \underset{M\to\infty}{\longrightarrow} \Phi_n^{LS\pi}, \quad E_n^{\rm PS} \underset{M\to\infty}{\longrightarrow} E_n^r \tag{8}$$

and that the method of Martín *et al.* provides the closed-channel wave function with a much more reduced computational effort.

B. Open-channel wave functions

The open-channel wave functions $\psi_\nu^+(E)$ are the solutions of

$$\left[E-P\mathcal{H}P-P\mathcal{H}Q\frac{1}{E-Q\mathcal{H}Q}Q\mathcal{H}P\right]\psi_\nu^+(E)=0 \tag{9}$$

with asymptotic conditions that depend on the physical situation considered (electron-atom scattering, photoionization, etc.[30,31]); ν represents the set of quantum numbers that identify a particular open channel. The total width is

$$\Gamma_n=\sum_\nu \Gamma_{n\nu} \ , \tag{10}$$

where

$$\Gamma_{n\nu}=2\pi|\langle\Phi_n^{LS\pi}|Q\mathcal{H}P|\psi_\nu^+\rangle|^2 \quad \text{for } E=E_n^r \tag{11}$$

is the ν partial width of the resonant state $\Phi_n^{LS\pi}$. The shift is given by

$$\delta E_n^r=\sum_\nu \delta E_{n\nu} \ , \tag{12}$$

where

$$\delta E_{n\nu}=\mathcal{P}\sum\!\!\!\!\!\!\int \frac{|\langle\Phi_n^{LS\pi}|Q\mathcal{H}P|\psi_\nu^+\rangle|^2}{(E_n^r-E')}dE' \ . \tag{13}$$

The symbol $\sum\!\!\!\!\!\!\int$ indicates integration over continuum states and summation over bound and resonant states below the N_t threshold, and $\mathcal{P}$ the principal value of the integral.

A general expansion of ψ_ν^+ must include all possible channels with the same symmetry as the closed-channel wave function $\Phi_n^{LS\pi}$, i.e., with the same L, S, π (and M_L, M_s) quantum numbers. Therefore, for a given set (L, S, π, M_L, M_S) we can write a general expansion for ψ_ν^+ of the type

$$\psi_\nu^{LS\pi^+}=\sum_{\gamma=1}^{N_t}\sum_{l_2}\Theta[\phi_\gamma(r_1)F_\gamma^{l_2}(r_2)\mathcal{J}_{l_1l_2}^{LM}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)] + \sum_k \Xi(\mathbf{r}_1,\mathbf{r}_2) \ , \tag{14}$$

where Θ is the symmetrization (for singlets) or antisymmetrization (for triplets) operator, l_2 is the angular momentum of the continuum orbital $F_\gamma^{l_2}$ and

$$\mathcal{J}_{l_1l_2}^{LM}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2) = \sum_{m_1,m_2}\langle l_1l_2m_1m_2|LM\rangle Y_{l_1}^{m_1}(\hat{\mathbf{r}}_1)Y_{l_2}^{m_2}(\hat{\mathbf{r}}_2) \ , \tag{15}$$

$$\Xi(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2) \underset{r_1,r_2\to\infty}{\longrightarrow} 0 \tag{16}$$

[$\Xi(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)$ can be bound and/or resonant states below the N_t threshold]. The summation over l_2 includes only the angular momenta of the continuum electrons that are consistent with the total angular momentum L. In the following, we will suppress the quantum numbers L, S, and π in both $\Phi_n^{LS\pi}$ and $\psi_\nu^{LS\pi^+}$. The insertion of Eq. (14) in Eq. (9) leads to a system of coupled differential equations. In practical calculations, however, one usually restricts the expansion (14) to a single term:[2,11,13,25–27]

$$\psi_{\alpha l}^{+} \simeq \chi_{\alpha l}(E) = \Theta[\phi_\alpha(r_l)F_\alpha^l(r_2)\mathcal{J}_{l_1 l_2}^{LM}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)] \tag{17}$$

which is a generalization of the static exchange approximation used in the one open-channel case.[32] This implies the solution of one uncoupled Schrödinger equation for each channel αl:

$$(E - P_\alpha \mathcal{H} P_\alpha)\chi_{\alpha l} = 0 \ , \tag{18}$$

where P_α is given by

$$P_\alpha = P_1^\alpha + P_2^\alpha - P_1^\alpha P_2^\alpha \ . \tag{19}$$

The use of these approximate continuum functions in Eqs. (10) and (11) has provided total widths Γ_n that are in reasonable agreement with results obtained with other theories.[25] Here we neglect the term $P\mathcal{H}Q(E - Q\mathcal{H}Q)^{-1}Q\mathcal{H}P$ in Eq. (9). The influence of this term has been initially discussed and calculated by Bhatia and Temkin.[32] The very small corrections due to this term involve couplings between open and closed channels; it seems reasonable then to neglect its contribution compared to $P_\alpha \mathcal{H} P_\beta$ terms which couple states with eventually large density overlap within the open-channel wave function (e.g., $2s\epsilon s$ and $2p\epsilon p$).

The theory we develop below will be applied in the next section to the study of the ${}^{1,3}S^e$ symmetry. In this particular case, the summation over l_2 contains only one term for each ϕ_γ orbital. Therefore, to identify each open channel is no longer necessary to maintain the index l in Eqs. (17) and (18). Then to simplify the notation we eliminate the index l in the following. For symmetries different from S^e, our development is still valid by adding such index whenever an open-channel wave function is involved.

Using Eqs. (3), (4), and (19), we can write the projected Hamiltonian $P\mathcal{H}P$ as

$$P\mathcal{H}P = H_0 + V_1 + V_2 + V_3 \ , \tag{20}$$

where

$$H_0 = \sum_\gamma P_\gamma \mathcal{H} P_\gamma \ , \tag{21}$$

$$V_1 = \sum_\sigma \sum_{\beta\neq\sigma} P_\sigma \mathcal{H} P_\beta \ , \tag{22}$$

$$V_2 = -\sum_\sigma \sum_\beta \sum_{\gamma\neq\beta} P_1^\beta P_2^\gamma \mathcal{H} P_\sigma - \sum_\sigma \sum_\beta \sum_{\gamma\neq\beta} P_\sigma \mathcal{H} P_1^\beta P_2^\gamma , \tag{23}$$

$$V_3 = \sum_\beta \sum_{\gamma\neq\beta} \sum_\sigma \sum_{\delta\neq\sigma} P_1^\beta P_2^\gamma \mathcal{H} P_1^\sigma P_2^\delta \ . \tag{24}$$

It can be easily shown that the eigensolutions χ_α of the uncoupled Schrödinger equation (18) verify

$$\left\langle \chi_\alpha(E) \,\middle|\, \sum_\gamma P_\gamma \mathcal{H} P_\gamma \,\middle|\, \chi_\alpha(E) \right\rangle = E + \sum_{\gamma\neq\alpha} O(S_{\gamma\alpha}^2) \ , \tag{25}$$

where $S_{\gamma\alpha}$ is the overlap

$$S_{\gamma\alpha} = \langle \phi_\gamma(\mathbf{r}) | F_{\alpha E}^l(r) Y_l^m(\hat{\mathbf{r}}) \rangle \ . \tag{26}$$

If we impose

$$S_{\gamma\alpha} \simeq 0 \quad \text{for } \gamma\neq\alpha \ , \tag{27}$$

the $\chi_\alpha(E)$ wave functions can be considered as zero-order functions in a perturbative treatment of $P\mathcal{H}P$ [Eq. (20)] with a zero-order Hamiltonian H_0 [Eq. (21)]. We will show in the next section that, in practice, Eq. (27) is almost directly verified by the χ_α obtained in a static exchange approximation and one does not need to impose such orthogonality condition. Therefore, we consider that the χ_α functions are orthogonal for different channels

$$\langle \chi_\alpha(E) | \chi_\beta(E) \rangle = O(S_{\alpha\beta} S_{\beta\alpha}) \simeq 0 \ . \tag{28}$$

A simple analysis shows that the contribution of V_2 and V_3 to the first-order correction of the χ_α wave functions is zero, since they involve terms $O(S_{\alpha\beta})$ with $\alpha\neq\beta$ and $O(S_{\alpha\beta}S_{\gamma\sigma})$ with $\alpha\neq\beta$ and $\gamma\neq\sigma$, respectively. Then, the remaining V_1 term is the only one responsible for the interaction between different open channels and the equation (9) can be written

$$\left[E - \sum_\gamma P_\gamma \mathcal{H} P_\gamma \right] \psi_\alpha^+(E) = \sum_{\substack{\sigma,\beta \\ \sigma\neq\beta}} P_\sigma \mathcal{H} P_\beta \psi_\alpha^+(E) \ . \tag{29}$$

Using the Lippman-Schwinger equation, we can formally write

$$\psi_\alpha^+(E) = \chi_\alpha(E) + \lim_{\epsilon\to 0+} \left[E - \sum_\gamma P_\gamma \mathcal{H} P_\gamma + i\epsilon \right]^{-1} \times \sum_{\substack{\sigma,\beta \\ \sigma\neq\beta}} P_\sigma \mathcal{H} P_\beta \psi_\alpha^+(E) \ . \tag{30}$$

A first-order treatment in V_1 leads to

$$\psi_\alpha^+(E) = \chi_\alpha(E) + \lim_{\epsilon\to 0+} \left[E - \sum_\gamma P_\gamma \mathcal{H} P_\gamma + i\epsilon \right]^{-1} \times \sum_{\sigma\neq\alpha} P_\sigma \mathcal{H} P_\alpha \chi_\alpha(E) \tag{31}$$

(for incoming waves the sign in $i\varepsilon$ is the opposite one, but that will not change our final result). Inserting in Eq. (31) the projection operator P:

$$P = \sum_\beta \sum\!\!\!\!\!\!\!\int |\chi_\beta(E')\rangle\langle\chi_\beta(E')| dE' \ , \tag{32}$$

we obtain, after some algebra,

$$\psi_\alpha^+(E)=\chi_\alpha(E)+\sum_{\sigma\neq\alpha}\mathcal{P}\,⨏\,dE'\frac{\langle\chi_\sigma(E')|P_\sigma\mathcal{H}P_\alpha|\chi_\alpha(E)\rangle}{(E-E')}\chi_\sigma(E')-i\pi\sum_{\sigma\neq\alpha}\langle\chi_\sigma(E)|P_\sigma\mathcal{H}P_\alpha|\chi_\alpha(E)\rangle\chi_\sigma(E)\;. \tag{33}$$

Then the partial width $\Gamma_{n\alpha}$ is up to first order in V_1:

$$\begin{aligned}\Gamma_{n\alpha}&=\Gamma^0_{n\alpha}+\Gamma^{(1)}_{n\alpha}\\&=2\pi|\langle\Phi_n|Q\mathcal{H}P_\alpha|\chi_\alpha(E)\rangle|^2\\&\quad+4\pi\langle\Phi_n|Q\mathcal{H}P_\alpha|\chi_\alpha(E)\rangle\sum_{\sigma\neq\alpha}\mathcal{P}\,⨏\,dE'\frac{\langle\chi_\sigma(E')|P_\sigma\mathcal{H}P_\alpha|\chi_\alpha(E)\rangle\langle\Phi_n|Q\mathcal{H}P_\sigma|\chi_\sigma(E')\rangle}{(E-E')}\;,\end{aligned} \tag{34}$$

where $\Gamma^0_{n\alpha}$ is the partial width obtained in the "uncoupled" approximation and $\Gamma^{(1)}_{n\alpha}$ is the correction derived from the interaction with channels different from α.

C. Discretization of continuum wave functions

To obtain both $\Gamma^0_{n\alpha}$ and $\Gamma^{(1)}_{n\alpha}$ we have to know only the $\chi_\alpha(E)$ functions for all the accessible open channels. We have solved Eq. (18) by using the discretization method of Macías *et al.*[8,10]. In this procedure, for each open channel α, the wave function χ_α is written, in the static exchange approximation, as a sum of configurations ξ^α_{jk} which are symmetry and spin projected of the form

$$\xi^\alpha_{jk}=\frac{N_{jk}}{\sqrt{2}}\Theta[\phi_\alpha(r_1)\bar{\phi}^j_k(r_2)\mathcal{J}^{LM}_{l_1l_2}(\hat{\mathbf{r}}_1,\hat{\mathbf{r}}_2)]\;, \tag{35}$$

where N_{jk} is the normalization factor and $\bar{\phi}^j_k$ are radial parts of Slater-type orbitals (STO's) whose exponents follow a geometrical sequence. The discretized function $\tilde{\chi}_\alpha(E)$ obtained in this way coincides with the δ-normalized $\chi_\alpha(E)$ function in a finite domain up to a normalization factor[10]

$$\chi_\alpha(E_n)\simeq\rho_\alpha^{1/2}(E_n)\tilde{\chi}_\alpha(E_n)\;, \tag{36}$$

where ρ_α is called density of states and is given by

$$\rho_\alpha(E_n)=\frac{2}{E_{n+1}-E_{n-1}}\;. \tag{37}$$

The resonant condition $E=E^r_n$ in Eq. (11) is achieved through an inverse interpolation procedure with respect to a common scaling factor introduced in the STO basis. Using Eq. (34) and the quadrature

$$\int dE'\to\sum_i\frac{(E_{i+1}-E_{i-1})}{2}=\sum_i\frac{1}{\rho(E_i)}\;, \tag{38}$$

the final expression for the partial width is

$$\Gamma^0_{n\alpha}=2\pi\rho_\alpha(E)|\langle\Phi_n|Q\mathcal{H}P_\alpha|\tilde{\chi}_\alpha(E)\rangle|^2\;, \tag{39}$$

$$\Gamma^{(1)}_{n\alpha}=4\pi\rho_\alpha(E)\langle\Phi_n|Q\mathcal{H}P_\alpha|\tilde{\chi}_\alpha(E)\rangle\sum_{\sigma\neq\alpha}\sum_{\substack{i\\E\neq E_i}}\frac{\langle\tilde{\chi}_\sigma(E_i)|P_\sigma\mathcal{H}P_\alpha|\tilde{\chi}_\alpha(E)\rangle\langle\Phi_n|Q\mathcal{H}P_\sigma|\tilde{\chi}_\sigma(E_i)\rangle}{(E-E_i)}\;. \tag{40}$$

The same quadrature (38) permits the evaluation of the shift[5]

$$\delta E^r_n=\sum_\alpha\sum_{\substack{k\\E^r_n\neq E_k}}\frac{|\langle\Phi_n|Q\mathcal{H}P_\alpha|\tilde{\chi}_\alpha(E_k)\rangle|^2}{(E^r_n-E_k)}\;. \tag{41}$$

III. RESULTS AND DISCUSSION

We have solved Eq. (6) for the $^{1,3}S^e(3lnl)$ resonant states of He, C^{4+}, N^{5+}, and O^{6+} in a representation of configurations built from the basis set of STO's given in Table I. We have used $M=500$ in the pseudopotential of Eq. (7) and we have checked that our results are invariant in the range $100\leq M\leq 1000$. We have also tested the convergence of our results by increasing the basis set, what did not change the resulting energies, and verifying that the weights of f^2 configuration in the closed-channel wave function are always ≤ 0.01 (except for the 5^1S^e state of He which is 0.05), so that contributions of higher-l quantum numbers cannot be expected.

The STO basis sets used in the solution of the open-channel equations (18) with the discretization procedure of Sec. II C are also given in Table I. For the S^e symmetry there are three open channels: $1s\epsilon s$, $2s\epsilon s$, and $2p\epsilon p$. The $2p\epsilon p$ continuum function is exactly orthogonal to the $1s\epsilon s$ and $2s\epsilon s$ ones. In Table II we give the overlaps between the $1s\epsilon s$ and $2s\epsilon s$ wave functions for N^{5+} at $E=E^r_n$. These results show that the orthogonality condition (28) is very well verified by our discretized continuum functions obtained in the static exchange approximation.

In Table III we present our calculated energies (with and without shift) for the first nine $^1S^e(3lnl)$ and first six $^3S^e(3lnl)$ resonant states of He, C^{4+}, N^{5+}, and O^{6+}, together with previous results of Ho and Callaway,[33] Oberoi,[34] Herrick and Sinanoglu,[27] Ormonde *et al.*[35] (for He), Ho,[36] Abu-Salbi and Callaway[1] (for C^{4+} and O^{6+}), Ho[7] and Oza *et al.*[16] (for N^{5+}), obtained with different approaches. Our unshifted energies for singlet and triplet states of He are in very good agreement with the results

TABLE I. Basis sets used in the calculations of the closed- and open-channel wave functions. The radial part of each STO is defined as $\bar{\phi}_k^j = A_{kj} r^{k-1} e^{-\alpha_j Z r}$. For the open-channel wave functions, α_0 represents the first exponent in the even-tempered sequence $\alpha_j = \alpha_0 \beta^{-j}$, with $j = 0, 1, \ldots, N-1$ and $\beta = 1.6$, of each ξ_{jk}^{α} configuration [see Eq. (35)].

Closed-channel wave function							
$l=0$		$l=1$		$l=2$		$l=3$	
k	α	k	α	k	α	k	α
1–3	$\frac{1}{3}$	2–3	$\frac{1}{3}$	3	$\frac{1}{3}$	4	$\frac{1}{4}$
4–6	$\frac{1}{5}$	4–6	$\frac{1}{5}$	3–6	$\frac{1}{5}$	4–6	$\frac{1}{5}$
7–9	$\frac{3}{20}$	7–9	$\frac{3}{20}$	7–9	$\frac{3}{20}$	7–9	$\frac{3}{20}$
10	$\frac{1}{10}$	10	$\frac{1}{10}$				
11	$\frac{1}{11}$						

Configurations included: all possible $nln'l$ with $n' < 7$
(138 configurations for singlets and 118 for triplets)

Open-channel wave functions								
$1s\epsilon s$			$2s\epsilon s$			$2p\epsilon p$		
k	α_0	N	k	α_0	N	k	α_0	N
2	$\frac{1}{2}$	9	2	$\frac{1}{2}$	9	2	$\frac{1}{2}$	9
4	$\frac{1}{4}$	9	4	$\frac{1}{4}$	9	4	$\frac{1}{4}$	9

Configurations included: all possible ξ_{jk}^{α} [Eq. (35)]

of Oberoi[34] who used a conventional Feshbach method and did not calculate the shifts. Our previous results for the two first $^1S^e$ resonances of N^{5+} reported in Ref. 25 are slightly improved since the present energies are obtained with a larger basis set. In order to compare with the results obtained with complex-scaling[7,33,36] or close-coupling[1,16,35] methods, we have also included the energy shift given in Eq. (41). In this case, the general agreement is also very good for all systems. The shift is always very small [$\simeq 10^{-4}$ for He and $\simeq 10^{-3}$ for C^{4+}, N^{5+}, and O^{6+}): one order of magnitude smaller than the experimental errors in electron spectroscopy experiments.

In Table IV we show the total widths of these resonant states calculated in the "uncoupled" approximation (Γ^0) and taking into account the interaction between different open channels ($\Gamma^0 + \Gamma^{(1)}$). These are compared with previous results.[1,7,16,27,33,35,36] For C^{4+}, N^{5+}, and O^{6+} our ($\Gamma^0 + \Gamma^{(1)}$) values are in excellent agreement with those of Ho,[7] Oza *et al.*[16] (N^{5+}), and Ho[36] and Abu-Salbi and Callaway[1] (C^{4+}, O^{6+}). This is very encouraging in view of the enormous basis set used by Ho[7,36] and the complexity of the close-coupling calculations.[1,16] However, even our "uncoupled" Γ^0 widths compare reasonably well to those results. In fact, Table IV shows that the $\Gamma^{(1)}$ corrections are always approximately one order of magnitude smaller than the corresponding Γ^0 widths. This last assertion is also valid for the He atom, although the comparison with other results for the singlet state is not so impressive as in the previous case. In this respect, we can observe in Table IV two major discrepancies for the widths of the $3\,^1S^e$ and $5\,^1S^e$ states. The disagreement for the $3\,^1S^e$ state (two orders of magnitude) concerns mainly the width reported by Ho and Callaway,[33] since our value is in fairly good agreement with the width reported by Ormonde *et al.*[35] and by Herrick and Sinanoglu.[27] In fact, as pointed out by Ho[36] this $3\,^1S^e$ resonant state of He is very unstable to variations in the parameters of the basis sets in a complex-scaling calculation. The value of our calculated width is more similar to that of the $4\,^1S^e$ state of the other three ions given in Table IV than to that of their $3\,^1S^e$ state. This has been explained by Bachau *et al.*[37] who proved that the correlations patterns are exchanged between the $3\,^1S^e$ and the $4\,^1S^e$ states for $Z > 2$.

The origin of the strong discrepancy for the width of the $5\,^1S^e$ state of He with the results of Ho and Callaway[33] and Herrick and Sinanoglu[27] is not as clear. In the work of Bachau *et al.*[37] it is also shown that the $4\,^1S^e$ and $5\,^1S^e$ resonances exchange abruptly their character and properties around $Z = 2$, in fact, when their energies are

TABLE II. Overlaps $\langle \chi_{1s\epsilon s}(E) | \chi_{2s\epsilon s'}(E) \rangle$ for N^{5+} between our discretized $\chi_{1s\epsilon s}$ and $\chi_{2s\epsilon s'}$ continuum wave functions at the resonance energies $E = E_n^r$ with $n = 1-10$.

	$\langle \chi_\alpha \vert \chi_\beta \rangle$		$\langle \chi_\alpha \vert \chi_\beta \rangle$
$1\,^1S^e$	7.54[−5]	$1\,^3S^e$	3.40[−7]
$2\,^1S^e$	7.21[−5]	$2\,^3S^e$	3.39[−7]
$3\,^1S^e$	6.67[−5]	$3\,^3S^e$	3.37[−7]
$4\,^1S^e$	5.87[−5]	$4\,^3S^e$	3.32[−7]
$5\,^1S^e$	5.73[−5]	$5\,^3S^e$	3.32[−7]
$6\,^1S^e$	5.57[−5]	$6\,^3S^e$	3.31[−7]
$7\,^1S^e$	5.35[−5]	$7\,^3S^e$	3.28[−7]
$8\,^1S^e$	5.29[−5]	$8\,^3S^e$	3.27[−7]
$9\,^1S^e$	5.22[−5]	$9\,^3S^e$	3.26[−7]
$10\,^1S^e$	5.11[−5]	$10\,^3S^e$	3.26[−7]

TABLE III. Energies of the first nine $^1S^e$ and first six $^3S^e$ resonant states of He, C^{4+}, N^{5+}, and O^{6+}, which lie above the $n=2$ threshold. $-E$: our calculated energies without shift; $-(E+\delta E)$: our results including the shift given in Eq. (41); O: results of Oberoi (Ref. 34); HC: results of Ho and Callaway (Ref. 33); HS: results of Herrick and Sinanoglu (Ref. 27); OWL: results of Ormonde *et al.* (Ref. 35); AC: results of Abu-Salbi and Callaway (Ref. 1); H: results of Ho (Refs. 7 and 36); O *et al.*: results of Oza *et al.* (Ref. 16).

			He			
	$-E$ (a.u.)	$-(E+\delta E)$ (a.u.)	O	HC	HS	OWL
$1\,^1S^e$	0.354 503	0.353 978	0.354 48	0.353 54	0.353 71	0.353 44
$2\,^1S^e$	0.316 450	0.316 683	0.316 14	0.317 45	0.313 69	0.316 66
$3\,^1S^e$	0.281 510	0.281 286	0.281 48	0.281 15	0.279 83	0.279 99
$4\,^1S^e$	0.263 503	0.262 970	0.263 04	0.263 50	0.261 34	0.261 67
$5\,^1S^e$	0.257 663	0.256 928	0.257 46	0.257 37	0.249 21	
$6\,^1S^e$	0.256 161	0.256 068	0.256 12		0.255 13	0.255 40
$7\,^1S^e$	0.246 610	0.246 483	0.246 38		0.245 67	0.246 29
$8\,^1S^e$	0.244 376	0.244 184	0.244 20		0.240 00	
$9\,^1S^e$	0.243 909	0.243 862	0.243 86		0.243 17	0.243 35
$1\,^3S^e$	0.287 343	0.287 277	0.287 34	0.287 28		
$2\,^3S^e$	0.270 364	0.270 260	0.270 36	0.270 28		
$3\,^3S^e$	0.258 163	0.258 135	0.258 14	0.258 13		
$4\,^3S^e$	0.250 034	0.249 934	0.250 02	0.249 96		
$5\,^3S^e$	0.249 009	0.248 984	0.249 00	0.249 00		
$6\,^3S^e$	0.244 819	0.244 805	0.244 82			

			C^{4+}	
	$-E$ (a.u.)	$-(E+\delta E)$ (a.u.)	AC	H
$1\,^1S^e$	3.714 438	3.712 520	3.7127	3.7127
$2\,^1S^e$	3.564 574	3.560 424	3.5619	3.5624
$3\,^1S^e$	3.289 262	3.281 642		3.2915
$4\,^1S^e$	2.911 376	2.910 417	2.9104	2.9106
$5\,^1S^e$	2.816 277	2.814 959	2.8136	2.8163
$6\,^1S^e$	2.695 590	2.692 882		
$7\,^1S^e$	2.569 512	2.569 097		
$8\,^1S^e$	2.518 248	2.517 719		
$9\,^1S^e$	2.457 144	2.455 737		
$1\,^3S^e$	2.937 301	2.937 202	2.9373	
$2\,^3S^e$	2.873 256	2.873 024	2.8729	
$3\,^3S^e$	2.766 421	2.765 897		
$4\,^3S^e$	2.578 860	2.578 844		
$5\,^3S^e$	2.540 581	2.540 469		
$6\,^3S^e$	2.487 185	2.486 923		

			N^{5+}	
	$-E$ (a.u.)	$-(E+\delta E)$ (a.u.)	O *et al.*	H
$1\,^1S^e$	5.109 799	5.107 727	5.1080	5.1080
$2\,^1S^e$	4.931 104	4.926 303	4.9275	4.9280
$3\,^1S^e$	4.601 278	4.592 926		4.6042
$4\,^1S^e$	4.002 701	4.001 656	4.002	4.0020
$5\,^1S^e$	3.888 029	3.886 434	3.885	3.8880
$6\,^1S^e$	3.739 585	3.736 523		
$7\,^1S^e$	3.525 553	3.525 101	3.524	
$8\,^1S^e$	3.463 838	3.463 204	3.462	
$9\,^1S^e$	3.389 342	3.387 803		
$1\,^3S^e$	4.033 775	4.033 673	4.035	
$2\,^3S^e$	3.957 938	3.957 692	3.958	
$3\,^3S^e$	3.829 738	3.829 162		
$4\,^3S^e$	3.536 804	3.536 749		
$5\,^3S^e$	3.491 131	3.491 008		
$6\,^3S^e$	3.426 510	3.426 220		

TABLE III. (*Continued*).

	$-E$ (a.u.)	$-(E+\delta E)$ (a.u.)	O^{6+} AC	H
$1\,^1S^e$	6.727 362	6.725 156	6.7254	6.7255
$2\,^1S^e$	6.519 716	6.514 360	6.5156	6.5168
$3\,^1S^e$	6.135 493	6.126 532		6.1390
$4\,^1S^e$	5.267 600	5.266 480	5.2669	5.2669
$5\,^1S^e$	5.133 265	5.131 436	5.1301	5.1332
$6\,^1S^e$	4.957 001	4.953 646		
$7\,^1S^e$	4.632 681	4.632 196		
$8\,^1S^e$	4.560 484	4.559 762		
$9\,^1S^e$	4.472 697	4.471 058		
$1\,^3S^e$	5.303 841	5.303 736	5.3037	
$2\,^3S^e$	5.216 213	5.215 953	5.2159	
$3\,^3S^e$	5.066 666	5.066 046		
$4\,^3S^e$	4.645 845	4.645 788		
$5\,^3S^e$	4.592 776	4.592 646		
$6\,^3S^e$	4.516 926	4.516 613		

TABLE IV. Total widths of the first nine $^1S^e$ and first six $^3S^e$ resonant states of He, C^{4+}, N^{5+}, and O^{6+}, which lie above the $n=2$ threshold. Γ^0: our results in the uncoupled approximation [Eqs. (10) and (39)]; $\Gamma^0+\Gamma^{(1)}$: our results including interaction between open channels [Eqs. (10), (39), and (40)]; HC: results of Ho and Callaway (Ref. 33); HS: results of Herrick and Sinanoglu (Ref. 27); OWL: results of Ormonde *et al.* (Ref. 35); AC: results of Abu-Salbi and Callaway (Ref. 1); H: results of Ho (Refs. 7 and 36); O *et al.*: results of Oza *et al.* (Ref. 16).

	Γ^0	$\Gamma^0+\Gamma^{(1)}$	He HC	HS	OWL
$1\,^1S^e$	0.0970	0.0800	0.0816	0.083	0.0860
$2\,^1S^e$	0.1709	0.1623	0.1810	0.146	0.2246
$3\,^1S^e$	0.0487	0.0407	0.0001	0.046	0.0478
$4\,^1S^e$	0.0573	0.0561	0.0639	0.037	0.0688
$5\,^1S^e$	0.0026	0.0017	0.0001	0.0003	
$6\,^1S^e$	0.0223	0.0189		0.023	0.0249
$7\,^1S^e$	0.0257	0.0251		0.018	0.0297
$8\,^1S^e$	0.0029	0.0024			
$9\,^1S^e$	0.0115	0.0130		0.015	
$1\,^3S^e$	0.0010	0.0008	0.0008		
$2\,^3S^e$	0.0013	0.0013	0.0013		
$3\,^3S^e$	0.0006	0.0005	0.0005		
$4\,^3S^e$	0.0004	0.0004	0.0001		
$5\,^3S^e$	0.0004	0.0004	0.0003		
$6\,^3S^e$	0.0004	0.0003			

	Γ^0	$\Gamma^0+\Gamma^{(1)}$	C^{4+} AC	H
$1\,^1S^e$	0.1453	0.1298	0.129	0.129
$2\,^1S^e$	0.5012	0.5271	0.524	0.525
$3\,^1S^e$	0.0065	0.0085		0.0078
$4\,^1S^e$	0.0895	0.0832	0.082	0.082
$5\,^1S^e$	0.2619	0.2703	0.276	0.276
$6\,^1S^e$	0.0026	0.0030		
$7\,^1S^e$	0.0428	0.0403		
$8\,^1S^e$	0.1268	0.1303		
$9\,^1S^e$	0.0014	0.0016		
$1\,^3S^e$	0.0015	0.0013	0.0013	
$2\,^3S^e$	0.0046	0.0047	0.0046	
$3\,^3S^e$	0.000 09	0.000 10		
$4\,^3S^e$	0.0012	0.0011		
$5\,^3S^e$	0.0035	0.0035		
$6\,^3S^e$	0.000 06	0.000 07		

TABLE IV. (*Continued*).

		N^{5+}		
	Γ^0	$\Gamma^0+\Gamma^{(1)}$	O *et al.*	H
$1\,^1S^e$	0.1495	0.1359	0.139	0.133
$2\,^1S^e$	0.5272	0.5523	0.544	0.571
$3\,^1S^e$	0.0061	0.0078		0.007
$4\,^1S^e$	0.0931	0.0876	0.087	0.088
$5\,^1S^e$	0.2820	0.2903	0.30	0.288
$6\,^1S^e$	0.0025	0.0028		
$7\,^1S^e$	0.0447	0.0426	0.041	
$8\,^1S^e$	0.1346	0.1384	0.14	
$9\,^1S^e$	0.0013	0.0014		
$1\,^3S^e$	0.0015	0.0014	0.0016	
$2\,^3S^e$	0.0049	0.0050	0.0049	
$3\,^3S^e$	0.000 09	0.000 10		
$4\,^3S^e$	0.0012	0.0012		
$5\,^3S^e$	0.0038	0.0038		
$6\,^3S^e$	0.000 06	0.000 07		
		O^{6+}		
	Γ^0	$\Gamma^0+\Gamma^{(1)}$	AC	H
$1\,^1S^e$	0.1532	0.1410	0.136	0.136
$2\,^1S^e$	0.5482	0.5723	0.579	0.569
$3\,^1S^e$	0.0059	0.0074		0.0069
$4\,^1S^e$	0.0961	0.0913	0.095	0.090
$5\,^1S^e$	0.2976	0.3057	0.313	0.305
$6\,^1S^e$	0.0024	0.0026		
$7\,^1S^e$	0.0461	0.0442		
$8\,^1S^e$	0.1405	0.1437		
$9\,^1S^e$	0.0012	0.0012		
$1\,^3S^e$	0.0015	0.0014	0.0015	
$2\,^3S^e$	0.0052	0.0053	0.0052	
$3\,^3S^e$	0.000 09	0.000 10		
$4\,^3S^e$	0.0013	0.0012		
$5\,^3S^e$	0.0040	0.0041		
$6\,^3S^e$	0.000 06	0.000 07		

TABLE V. Partial widths of the first nine $^1S^e$ and first six $^3S^e$ resonant states of He, C^{4+}, N^{5+}, and O^{6+}, which lie above the $n=2$ threshold. Γ^0_α: our results in the uncoupled approximation [Eq. (39)]; $\Gamma^{(1)}_\alpha$: corrections due to the interaction between open channels [Eq. (40)]. Numbers in square brackets denote powers of 10 by which the preceding value should be multiplied.

			He			
	$\Gamma^0_{1s\epsilon s}$	$\Gamma^{(1)}_{1s\epsilon s}$	$\Gamma^0_{2s\epsilon s}$	$\Gamma^{(1)}_{2s\epsilon s}$	$\Gamma^0_{2p\epsilon p}$	$\Gamma^{(1)}_{2p\epsilon p}$
$1\,^1S^e$	5.98[−3]	−2.40[−3]	6.75[−2]	2.81[−3]	2.36[−2]	−1.74[−2]
$2\,^1S^e$	1.38[−6]	−3.99[−5]	2.53[−2]	−7.87[−3]	1.45[−1]	−6.97[−4]
$3\,^1S^e$	3.61[−3]	−9.79[−4]	3.39[−2]	−5.71[−4]	1.12[−2]	−6.41[−3]
$4\,^1S^e$	6.43[−6]	5.02[−5]	9.33[−3]	−2.49[−3]	4.80[−2]	1.19[−3]
$5\,^1S^e$	3.99[−5]	1.75[−5]	4.33[−6]	3.71[−5]	2.59[−3]	−9.41[−4]
$6\,^1S^e$	1.73[−3]	−4.32[−4]	1.53[−2]	−3.38[−4]	5.31[−3]	−2.64[−3]
$7\,^1S^e$	2.00[−6]	1.72[−5]	4.03[−3]	−8.49[−4]	2.17[−2]	1.81[−4]
$8\,^1S^e$	1.71[−5]	1.29[−6]	8.74[−5]	9.88[−5]	2.84[−3]	−6.13[−4]
$9\,^1S^e$	9.05[−4]	−2.09[−4]	7.92[−3]	−2.28[−4]	2.67[−3]	−1.26[−3]
$1\,^3S^e$	1.85[−6]	−4.74[−7]	5.56[−4]	−6.35[−5]	4.24[−4]	−8.36[−5]
$2\,^3S^e$	3.49[−12]	4.54[−10]	2.39[−4]	2.32[−5]	1.09[−3]	−3.61[−5]
$3\,^3S^e$	1.37[−6]	−3.26[−7]	3.37[−4]	−3.79[−5]	2.57[−4]	−4.65[−5]
$4\,^3S^e$	2.67[−9]	7.72[−9]	7.31[−5]	2.79[−6]	3.10[−4]	−7.85[−7]
$5\,^3S^e$	1.67[−9]	−4.99[−9]	6.44[−5]	7.81[−6]	3.33[−4]	−2.01[−5]
$6\,^3S^e$	8.38[−7]	−1.86[−7]	2.35[−4]	−2.28[−5]	1.38[−4]	−2.47[−5]

TABLE V. (*Continued*).

C^{4+}

	$\Gamma^0_{1s\epsilon s}$	$\Gamma^{(1)}_{1s\epsilon s}$	$\Gamma^0_{2s\epsilon s}$	$\Gamma^{(1)}_{2s\epsilon s}$	$\Gamma^0_{2p\epsilon p}$	$\Gamma^{(1)}_{2p\epsilon p}$
$1\,^1S^e$	1.08[−2]	5.09[−4]	6.62[−2]	−1.48[−2]	6.38[−2]	−1.18[−3]
$2\,^1S^e$	1.22[−7]	−3.59[−6]	7.61[−2]	3.30[−2]	4.25[−1]	−7.09[−3]
$3\,^1S^e$	1.69[−4]	1.76[−5]	3.52[−3]	5.69[−4]	2.84[−3]	1.39[−3]
$4\,^1S^e$	8.16[−3]	3.91[−4]	3.96[−2]	−7.50[−3]	4.17[−2]	8.28[−4]
$5\,^1S^e$	1.84[−6]	−1.06[−5]	3.80[−2]	1.35[−2]	2.24[−1]	−5.00[−3]
$6\,^1S^e$	1.00[−4]	1.61[−5]	1.53[−3]	−5.90[−5]	1.01[−3]	4.35[−4]
$7\,^1S^e$	4.03[−3]	1.98[−4]	1.78[−2]	−3.30[−3]	2.10[−2]	5.89[−4]
$8\,^1S^e$	3.49[−6]	−1.01[−5]	1.85[−2]	6.00[−3]	1.08[−1]	−2.49[−3]
$9\,^1S^e$	6.29[−5]	1.08[−5]	8.47[−4]	−8.93[−5]	5.25[−4]	2.14[−4]
$1\,^3S^e$	4.60[−6]	−1.47[−7]	5.99[−4]	−7.20[−5]	8.53[−4]	−3.98[−5]
$2\,^3S^e$	1.30[−8]	3.10[−9]	9.84[−4]	1.35[−4]	3.59[−3]	−4.66[−5]
$3\,^3S^e$	1.06[−7]	2.99[−9]	3.73[−5]	2.72[−6]	4.97[−5]	9.58[−6]
$4\,^3S^e$	4.22[−6]	−1.42[−7]	4.97[−4]	−5.28[−5]	6.92[−4]	−2.58[−5]
$5\,^3S^e$	9.87[−9]	3.36[−9]	7.32[−4]	8.57[−5]	2.73[−3]	−4.07[−5]
$6\,^3S^e$	1.05[−7]	3.46[−9]	2.76[−5]	5.79[−7]	3.25[−5]	6.13[−6]

N^{5+}

	$\Gamma^0_{1s\epsilon s}$	$\Gamma^{(1)}_{1s\epsilon s}$	$\Gamma^0_{2s\epsilon s}$	$\Gamma^{(1)}_{2s\epsilon s}$	$\Gamma^0_{2p\epsilon p}$	$\Gamma^{(1)}_{2p\epsilon p}$
$1\,^1S^e$	1.12[−2]	5.74[−4]	6.59[−2]	−1.40[−2]	7.23[−2]	−1.76[−4]
$2\,^1S^e$	3.85[−7]	−6.70[−6]	8.21[−2]	3.21[−2]	4.45[−1]	−7.05[−3]
$3\,^1S^e$	1.80[−4]	9.77[−6]	3.70[−3]	5.53[−4]	2.27[−3]	1.13[−3]
$4\,^1S^e$	8.56[−3]	3.99[−4]	3.98[−2]	−7.03[−3]	4.47[−2]	1.17[−3]
$5\,^1S^e$	3.27[−6]	−1.44[−5]	4.17[−2]	1.31[−2]	2.40[−1]	−4.77[−3]
$6\,^1S^e$	1.15[−4]	1.35[−5]	1.64[−3]	−8.07[−5]	7.55[−4]	3.45[−4]
$7\,^1S^e$	4.23[−3]	1.99[−4]	1.78[−2]	−3.07[−3]	2.26[−2]	7.19[−4]
$8\,^1S^e$	5.62[−6]	−1.28[−5]	2.01[−2]	5.70[−3]	1.14[−1]	−2.32[−3]
$9\,^1S^e$	7.06[−5]	9.29[−6]	8.74[−4]	−1.01[−4]	3.58[−4]	1.60[−4]
$1\,^3S^e$	4.88[−6]	−1.17[−7]	5.96[−4]	−6.55[−5]	8.96[−4]	−3.41[−5]
$2\,^3S^e$	1.69[−8]	1.74[−9]	1.07[−3]	1.32[−4]	3.84[−3]	−4.31[−5]
$3\,^3S^e$	1.21[−7]	1.48[−9]	4.06[−5]	2.78[−6]	4.96[−5]	8.95[−6]
$4\,^3S^e$	4.54[−6]	−1.17[−7]	5.00[−4]	−4.85[−5]	7.39[−4]	−2.22[−5]
$5\,^3S^e$	1.33[−8]	2.52[−9]	8.09[−4]	8.47[−5]	2.97[−3]	−3.82[−5]
$6\,^3S^e$	1.26[−7]	2.32[−9]	3.01[−5]	5.58[−7]	3.19[−5]	5.68[−6]

O^{6+}

	$\Gamma^0_{1s\epsilon s}$	$\Gamma^{(1)}_{1s\epsilon s}$	$\Gamma^0_{2s\epsilon s}$	$\Gamma^{(1)}_{2s\epsilon s}$	$\Gamma^0_{2p\epsilon p}$	$\Gamma^{(1)}_{2p\epsilon p}$
$1\,^1S^e$	1.16[−2]	5.52[−4]	6.60[−2]	−1.31[−2]	7.56[−2]	4.33[−4]
$2\,^1S^e$	6.87[−7]	−8.97[−6]	8.71[−2]	3.09[−2]	4.61[−1]	−6.83[−3]
$3\,^1S^e$	1.89[−4]	4.19[−6]	3.88[−3]	5.22[−4]	1.89[−3]	9.38[−4]
$4\,^1S^e$	8.88[−3]	3.92[−4]	4.01[−2]	−6.59[−3]	4.72[−2]	1.35[−3]
$5\,^1S^e$	4.75[−6]	−1.70[−5]	4.48[−2]	1.26[−2]	2.53[−1]	−4.49[−3]
$6\,^1S^e$	1.27[−4]	1.13[−5]	1.74[−3]	−9.98[−5]	5.76[−4]	2.77[−4]
$7\,^1S^e$	4.39[−3]	1.94[−4]	1.79[−2]	−2.86[−3]	2.38[−2]	7.81[−4]
$8\,^1S^e$	7.73[−6]	−1.45[−5]	2.13[−2]	5.36[−3]	1.19[−1]	−2.14[−3]
$9\,^1S^e$	7.62[−5]	7.97[−6]	8.85[−4]	−1.10[−4]	2.43[−4]	1.19[−4]
$1\,^3S^e$	5.10[−6]	−9.45[−8]	5.94[−4]	−5.99[−5]	9.32[−4]	−2.98[−5]
$2\,^3S^e$	2.05[−8]	6.33[−10]	1.14[−3]	1.28[−4]	4.04[−3]	−3.97[−5]
$3\,^3S^e$	1.35[−7]	3.88[−10]	4.32[−5]	2.75[−6]	4.95[−5]	8.33[−6]
$4\,^3S^e$	4.78[−6]	−9.80[−8]	5.02[−4]	−4.47[−5]	7.77[−4]	−1.95[−5]
$5\,^3S^e$	1.66[−8]	1.77[−9]	8.72[−4]	8.23[−5]	3.16[−3]	−3.56[−5]
$6\,^3S^e$	1.44[−7]	1.44[−9]	3.21[−5]	5.10[−7]	3.14[−5]	5.25[−6]

represented as functions of Z, they present an avoided crossing in that region. Therefore, any small deficiency in the basis sets used in the calculations would appreciably affect the widths of these states of He, especially in this case where two states with quite different widths are mixed. On the other hand, the $5\,^1S^e$ state is very unstable in complex-scaling calculations[36] with respect to small variations in the rotation angle; also, the set of configurations used by Herrick and Sinanoglu[27] is too restrictive since it only includes $3lnl$ configurations.

Finally, in Table V we present the partial widths Γ_α^0 obtained in the "uncoupled" approximation and the corresponding $\Gamma_\alpha^{(1)}$ corrections due to the interaction between the different open channels. In this case, there is neither theoretical nor experimental data available to compare with. It is apparent from Table V that, in general, for C^{4+}, N^{5+}, and O^{6+} the $\Gamma_\alpha^{(1)}$ corrections are much smaller than the zero-order approximations $\Gamma_\alpha^{(0)}$, especially for triplet states. For singlet resonances, these corrections are slightly more important: in the most unfavorable cases, they do not exceed 35% of Γ_α^0 (the very small widths are excluded in this analysis). For the He atom, we can state the same qualitative argument, although the previous percentage would have to be slightly increased in some isolated cases.

IV. CONCLUSIONS

We have presented, in the framework of the Feshbach formalism, a simple perturbative method to calculate total and partial widths of atomic resonances above more than one ionization threshold that takes into account the interaction between different open channels. We have shown that the accuracy of the total widths obtained in this way is comparable to that provided by other methods such as complex scaling or close coupling. Besides, it provides directly partial widths that would be hard to obtain with other different approaches. Its computational implementation is very easy when it is combined with the pseudopotential Feshbach method of Martín *et al.*[11,12] which avoids solving a projected Schrödinger equation in the closed-channel space, and the discretization procedure of Macías *et al.*[8,10] is used to calculate the open-channel components. Indeed, for a given basis in our pseudopotential approach, the set of dielectronic integrals does not depend on the number of ionization thresholds involved, so that computer times to obtain the resonance wave functions are the same than those required for the calculation of bound states with such a basis. This is no longer true when projection of nonhydrogenic basis sets is used in the standard Feshbach approach. Moreover, the evaluation of partial and total widths with both our discretization and perturbative methods require computer times which are comparable to those involved in the evaluation of widths for resonant states which lie above only one ionization threshold.[38] This computer saving is larger when our comparison is carried out with other nonFeshbach methods.

We have analyzed the neglect of the interaction between different open-channels in the calculation of the continuum wave functions. The relative errors originated by such an approximation are always small for total and partial widths. The physical reason is that transition amplitudes for electron-ion inelastic scattering are always small at resonance energies as compared to the unity amplitudes corresponding to the initial condition in one specific channel. This also shows the validity of the static exchange approximation in the case of several open channels. The method proposed to calculate corrections to this "uncoupled" approximation has been easily applied in the framework of the discretization method of Macías *et al.*[8,10] The resulting corrected widths are comparable to those obtained through much more ellaborate methods from the computational point of view. Our work illustrates the efficiency of the Feshbach method to give accurate energies and widths of resonant states which lie above several ionization thresholds.

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