Feshbach-model potential approach for the study of resonant and bound states of Be-like ions

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We present an implementaion of the Feshbach formalism to calculate energy positions and widths of doubly excited states of Be-like ions. These systems can be treated formally as two-electron problems by using a suitable model potential to describe the effect of the $1s^2$ core. In this respect, we discuss the pertinence of using the one-parameter model potential $V_m = 2r^{-1} - 2r^{-1}(1+ar)e^{-2ar}$. Energies and widths for $1s^2 4l 4l'$ $^1S^e$ and $^1P^o$ autoionizing states of N^{3+} and Ne^{6+} are reported.

I. INTRODUCTION

Resonant and bound two-valence-electron states outside a $1s^2$ core have received particular attention in the last years. The interest for such systems has been spurred by the increasing experimental work in the formation of doubly excited states in collisions between multicharged ions and gaseous targets.[1-5] One major difficulty for the experimentalists is the lack of knowledge of the energy levels and partial widths of the resonant states, especially for multicharged ions. In the case of heliumlike ions many calculations have been performed. In particular it has been shown, in a recent work, that the Feshbach formalism[6] provides results which permit the interpretation of the experimental spectrum.[7] This is very interesting in view of the versatility of this method which allows to calculate partial widths, energies, and structure of resonant states.

Recently Martín et al[8] have proposed a generalization of the Feshbach method to the study of $1s^2 nln'l'$ doubly excited states of Be-like systems, where the effect of the $1s^2$ core is represented by a model potential V_m. The use of model potentials for the description of "passive" electrons in atomic and molecular systems is a topic that has received continuous attention from the beginning of atomic and molecular physics (see, for example, Refs. 9–11). They not only provide a much simpler way to study many electron systems that would be scarce with fully *ab initio* techniques, but are also useful in understanding the physical interpretation of phenomena in which a reduced number of electrons are involved. In dynamical processes such as atomic collisions, electron-atom collisions, etc., generally a reduced number of electrons are active and the remaining ones play an almost passive role. Then, the use of a model Hamiltonian for the active electrons, which includes the average effect of the passive ones, seems to be a good description. The use of a unique form for this averaged potential, which can describe all the states of the active electrons, greatly simplifies the treatment. This picture is not restricted to the study of processes in which only bound states are involved. We analyze, in this paper, how a model potential can also be used to describe resonant states with an inner core.

As this paper is devoted to the study of doubly excited states with the Feshbach approach, one has to analyze how the same potential V_m may be used to represent the "$1s^2 + 1$ electron" states (which are used to build the projection operator P) and the doubly excited states $1s^2 nln'l'$ consistently. We shall justify and analyze the degree of approximation involved in our "Feshbach-model potential" approach. The basic problem in all these studies is to find an analytical expression for the model potential which accounts for the intershell interactions. We will consider in this paper only the nonrelativistic limit and, consequently, a nuclear charge smaller, or equal to, 10 a.u. As the interpretation of the spectrum obtained by electron spectroscopy experiences requires an absolute precision of 0.1–0.2 eV for the theoretical energies, our goal is to provide results whose accuracy lies within this range.

In a first step, the "one-active electron" problem is solved in order to define V_m and the P operator (Sec. II). Then the "two-active electron" case will be considered (Sec. III). Although our interest concerns mainly the case of multicharged ions, most of the comparisons will be made with Li, Be, Be$^+$ (which are "unfavorable" cases for us) for which most of the calculations have been performed until now.

Atomic units will be used throughout, unless otherwise stated.

II. ONE ELECTRON IN THE FIELD OF A $1s^2$ CORE

A. The model potential

A number of analytical model potentials have been proposed in the literature (for a review of them, see, for example, Ref. 10). A simple one is given by the electrostatic potential produced by a nucleus of charge Z and two $1s$ electrons

$$V(r) = -\frac{Z}{r} + V_m(r) \tag{1}$$

with V_m a (model) potential of the form

$$V_m(r) = \frac{2}{r} - \frac{2}{r}(1+ar)e^{-2ar} , \tag{2}$$

where α is the effective charge felt by the two electrons described by $1s$ orbitals $(\alpha \simeq Z)$. This function verifies the correct asymptotic conditions

$$V(r) \underset{r \to \infty}{\sim} -\frac{Z-2}{r} \ , \tag{3}$$

$$V(r) \underset{r \to 0}{\sim} -\frac{Z}{r} \ . \tag{4}$$

The model potential defined in Eq. (2) has been widely used to calculate bound states of three- and four-electron systems (see, for example, Ref. 12 and references therein). In these works, the parameter α is fitted to reproduce the experimental energy of the $^2S(1s^22s)$ ground state and the corresponding model potential is used to calculate their excited states as well as the ground or excited states of the four-electron system. In all cases the results are in agreement with the experimental data or with more elaborate calculations. Unfortunately, this agreement has been stated as an empirical fact and there is no rigorous quantitative justification for it.

In the Hartree-Fock (HF) approach the wave function for a valence electron in the presence of a $1s^2$ core is the solution of

$$[h_{HF}(i) - \varepsilon_v]\phi_v(r_i) = 0 \tag{5}$$

with

$$h_{HF}(i) = -\tfrac{1}{2}\nabla_i^2 - \frac{Z}{r_i} + 2V^d(r_i) - V^{ex}(r_i) \ , \tag{6}$$

where $V^d(r_i)$ and $V^{ex}(r_i)$ are the usual direct and (nonlocal) exchange potentials, respectively,

$$V^d(r_i)\phi_v(r_i) = \langle \phi_{1s}(r_j)|r_{ij}^{-1}|\phi_{1s}(r_j)\rangle_{r_j}\phi_v(r_i) \tag{7}$$

$$V^{ex}(r_i)\phi_v(r_i) = \langle \phi_{1s}(r_j)|r_{ij}^{-1}|\phi_v(r_j)\rangle_{r_j}\phi_{1s}(r_i) \tag{8}$$

and the subscript r_j indicates that the integration must be done over this coordinate. In a first-order approximation, we can use hydrogenic functions to describe the frozen $1s^2$ core and the valence electron. Then, the direct term takes the well-known form

$$2V^d(r_i) = \frac{2}{r_i} - \frac{2}{r_i}(1 + Zr_i)e^{-2Zr_i} \tag{9}$$

which is formally equivalent to the electrostatic potential of Eq. (2) with $\alpha = Z$. We could better describe the $1s^2$ core by using hydrogenic orbitals with an effective charge
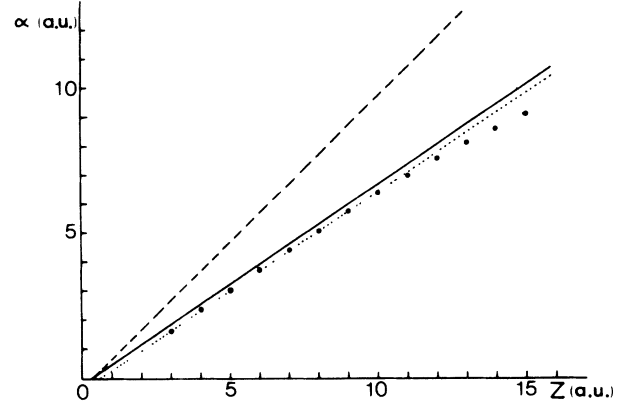

FIG. 1. Plot of the α parameter [see Eq. (2)] vs the nuclear charge Z. ($\bullet$) α^{expt} obtained by fitting the second eigenvalue of Eq. (11) to the $^2S(1s^22s)$ experimental energy (Ref. 15) ($\cdot \ \cdot \ \cdot \ \cdot$) fit of the previous values for $Z \le 10$ [see Eq. (18)]; ($- - -$) α values obtained when only the direct potential V^d is considered [Eq. (10) with $\sigma = \tfrac{5}{16}$]; ($———$) α values obtained when both direct V^d and exchange V^{ex} potentials are considered [Eq. (17)].

$Z_e = Z - \sigma$; the minimum energy for the core electrons is obtained for $\sigma = \tfrac{5}{16}$. Then, in general,

$$\alpha = Z - \sigma \ . \tag{10}$$

The electrostatic model that is used to justify Eq. (2) corresponds to the direct potential in the Hartree-Fock equations.

Here, we determine the parameter α by fitting the second lowest eigenvalue of the Schrödinger equation:

$$(H_m - E)\phi_{nl} = 0 \ , \tag{11}$$

where

$$H_m = -\tfrac{1}{2}\nabla^2 - \frac{Z}{r} + V_m(r) \tag{12}$$

to the experimental energy of the $^2S(1s^22s)$ ground state [the lowest eigenvalue is associated to the $^2S(1s^21s)$ virtual state]. The resulting values α^{expt} (Fig. 1) differ from those given in Eq. (10). The α^{expt} values follow a straight line for nuclear charges $Z \lesssim 10$ a.u., but the slope is quite different from that of Eq. (10). This difference can be allotted to the exchange potential.

To illustrate this point, let us consider the $1s^22s$ and $1s^22p$ states. We approximate the exchange potentials by

$$V_{2s}^{ex}(r) \simeq \frac{\langle \Phi_{1s}|r_{ij}^{-1}|\Phi_{2s}\rangle \Phi_{1s}(r)}{\Phi_{2s}(r)} = \frac{32 + 48Z_e r}{27(2 - Z_e r)}Z_e e^{-2Z_e r} \ , \tag{13}$$

$$V_{2p}^{ex}(r) \simeq \frac{\langle \Phi_{1s}|r_{ij}^{-1}|\Phi_{2p}\rangle \Phi_{1s}(r)}{\Phi_{2p}(r)} = e^{-Z_e r/2}\frac{1024}{243Z_e^2 r^3} - 16e^{-2Z_e r}\left[\frac{Z_e}{9} + \frac{8}{27r} + \frac{32}{81Z_e r^2} + \frac{64}{243Z_e^2 r^3}\right] \ , \tag{14}$$

where Φ_{nl} are hydrogenic wave functions calculated with a nuclear charge Z_e.

These potentials are represented in Fig. 2 for the Be$^+$ ion. It must be noticed that the exchange potential for

the $2s$ orbital presents a singularity at $r = 2/Z_e$, while the $2p$ one does not. This is a well-known effect[13] for all the orbitals with $n \ne l + 1$, resulting from the approximation used to represent the exchange potential. However, we
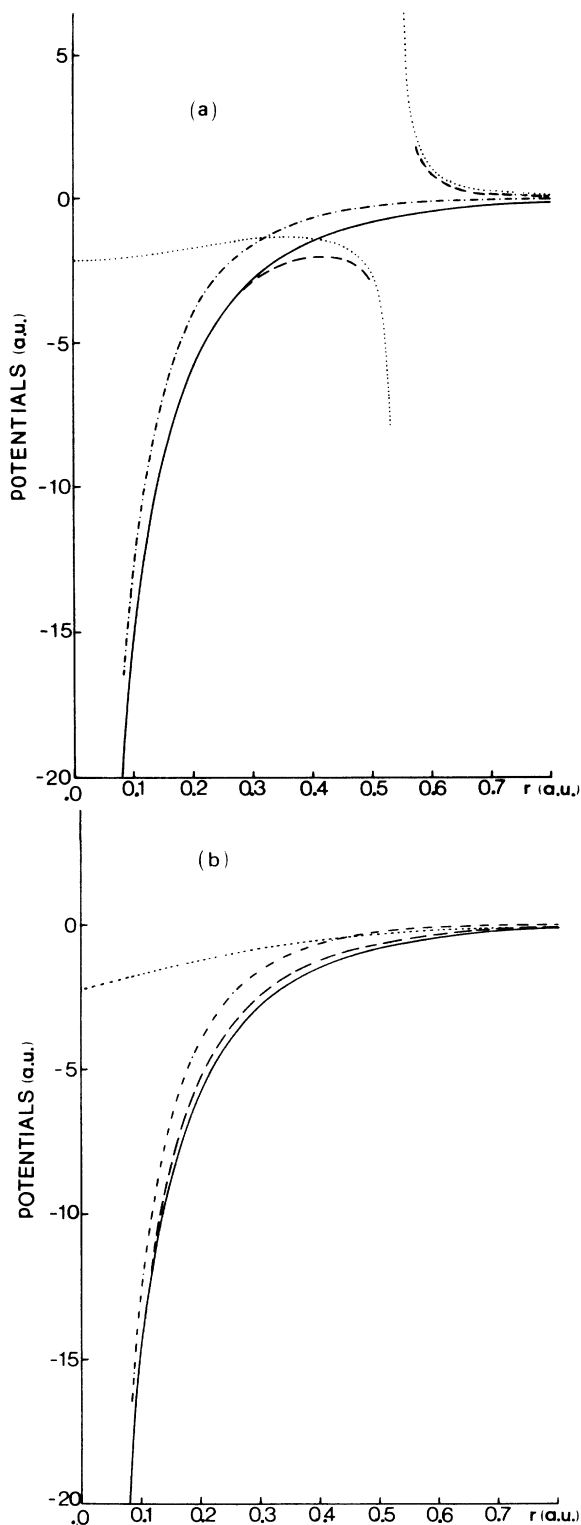
FIG. 2. Comparison between the model potential V_m (——)
of Eq. (2) with $\alpha = 2.333\,710$ [which fits the second eigenvalue of
Eq. (11) to the $^2S(1s^22s)$ experimental energy of Be$^+$] and (a)
(— · — · —·) the direct potential $2V^d$ of Eq. (9); (· · · ·) the ex-
change potential $-V_{2s}^{ex}$ of Eq. (13); (— — —) $2V^d - V_{2s}^{ex}$; (b)
(— · — · —·) the direct potential $2V^d$ of Eq. (9); (· · · ·) the ex-
change potential $-V_{2p}^{ex}$ of Eq. (14); (— — —) $2V^d - V_{2p}^{ex}$; for
$Z=4$ and $\sigma = \frac{5}{16}$. In both figures the term $2/r$ has been re-
moved from V_m and $2V^d$. r is the distance to the nucleus.

can use it in the region of small r, where the exchange
with the core electrons is more important. In Fig. 2 we
have also drawn the direct potential defined in Eq. (9) for
the effective charge Z_e, and the model potential V_m [Eq.
(2)] obtained with the value α^{expt}. To make this compar-
ison more apparent, in both cases we have suppressed the
common $2/r$ term. It can be seen that the direct poten-
tial $2V^d$ is substantially different from the model poten-
tial that gives the correct ground-state energy. However,
when the exchange potentials of Eqs. (13) and (14) are
added to $2V^d$, the resulting $2V^d - V_{nl}^{ex}$ potentials coincide
with V_m in the region $r \lesssim Z_e^{-1}$, where the core electrons
are present. As a consequence, the fitted model poten-
tials V_m correctly account for the exchange potentials of
the $2s$ and $2p$ orbitals. This qualitative observation can
be justified quantitatively by an analytical development of
the HF model potential:

$$V_m \equiv 2V^d - V^{ex} \tag{15}$$

in the core region ($r \to 0$). Using (A3) of Appendix A
that gives $V_{nl}^{ex}(r=0)$ for the exchange potential of a Φ_{nl}
orbital, the identity (15) becomes

$$2\alpha_{2s,2p} = 2Z_e - V_{nl}^{ex}(r=0) = 2Z_e - \tfrac{16}{27}Z_e \tag{16}$$

for both $2s$ and $2p$ orbitals. For the effective charge
$Z_e = Z - \tfrac{5}{16}$ mentioned above

$$\alpha_{2s,2p} = \tfrac{19}{27}Z - \tfrac{95}{432} \simeq 0.7Z - 0.2 \tag{17}$$

which is also shown in Fig. 1. It can be seen in this figure
that this equation agrees fairly well with the empirical
law

$$\alpha^{expt} \simeq 0.7Z - 0.4 \tag{18}$$

The departure from this behavior for higher values of
Z ($Z > 10$) is due to the increasing importance of relativ-
istic effects. In fact, the relativistic effects increase as Z^4
and are particularly important for the core electrons. We
have checked, by using an independent electron model
and the hydrogenic relativistic corrections to the energy,
that the linear behavior is present when these relativistic
contributions are removed.

Another important consequence of Figs. 1 and 2 is that
the exchange potential is the same for the $2s$ and $2p$ orbit-
als in the limit $r = 0$ and very similar in the core region.
This justifies that an l-independent model potential can
give a simultaneous good description of both.

We now discuss the appropriateness of V_m [Eq. (2)] to
obtain more excited states. Considering V^{ex} as a pertur-
bation, it is easy to show that, for highly excited states,
the first-order correction to the energy $E_{ex}^{(1)}$ produced by
the exchange potentials varies as[14]

$$E_{ex}^{(1)} \sim Zn^{-3} . \tag{19}$$

Therefore, for $n \gg 1$, the exchange potential can be
neglected and even a bad description of it does not affect
the energies of highly excited states. However, for
moderate values of n ($n > 2$), a bad description of the ex-
change, potential could lead to important errors. Then it
is worth estimating these exchange potentials for every

TABLE I. STO basis set used in the calculations of the wave functions in Eqs. (11) and (25). The definition of each STO is $\phi_{nlm}(r)=N_{nl}r^{n-1}e^{-(Z-1.7)\xi_l r}Y_l^m(\theta,\varphi)$.

$l=0$		$l=1$		$l=2$		$l=3$	
n	ξ_l	n	ξ_l	n	ξ_l	n	ξ_l
1	1						
1–2	$\frac{1}{2}$	2	$\frac{1}{2}$				
1–3	$\frac{1}{3}$	2–3	$\frac{1}{3}$	3	$\frac{1}{3}$		
4–6	$\frac{1}{4}$	4–6	$\frac{1}{4}$	4–6	$\frac{1}{4}$	4	$\frac{1}{4}$
7–9	$\frac{1}{7}$	7–9	$\frac{1}{7}$	7–9	$\frac{1}{7}$	5–7	$\frac{1}{5}$

orbital. This has been done in Appendix A in the limit $r \rightarrow 0$. It can be seen there that, for the $3s$, $3p$, and $3d$ orbitals, the exchange potential differs only slightly from the exchange potential associated with the $2s$ and $2p$ orbitals.

B. Calculations

We have calculated the eigenenergies and eigenfunctions of the one-electron Schrödinger equation (11) in the

representation of Slater-type orbitals (STO) in Table I. This basis set can be considered as complete to represent orbitals with $n \leq 4$. In Table II we show the energies for the $Be^+(1s^2nl)$ and $Ne^{7+}(1s^2nl)$ systems calculated with $\alpha=2.333\,710$ and $6.366\,365$, respectively, chosen to exactly reproduce the $^2S(1s^22s)$ ground states. For comparison, this table also includes the corresponding $1s^2nl$ experimental energies[15] and some other results[16,17] obtained with different model potential approaches for Be^+. It can be observed that for Be^+ the difference between

TABLE II. Energies for the $1s^2nl$ states of Be^+ and Ne^{7+} ions obtained with $\alpha=2.333\,710$ and $\alpha=6.366\,365$, respectively, and the basis set of Table I. Comparison with previous calculations. The experimental data are taken from Ref. 15. All the values are referred to the $X^{(Z-2)+}(1s^2)$ core energy. $|\Delta E|$ is the absolute value of the difference between our results and the experimental ones. The first-order correction $E_{nl}^{(1)}$ has been calculated according to Eq. (B4) of Appendix B with α_{nl} given in Eq. (B3), except those indicated by an asterisk which have been evaluated with α_{2p} of Eq. (B6).

				$-E$ (a.u.)			
nl	Our result	Expt. (Ref. 15)	$|\Delta E|$	$|E_{nl}^{(1)}|$	Laughlin et al. (Ref. 16)	Lin (Ref. 17)
				Be^+			
$2s$	0.669 248	0.669 246	0.000 002		0.669 18	0.6697
$3s$	0.267 685	0.267 233	0.000 452	6×10^{-4}	0.267 39	0.237 35
$4s$	0.143 381	0.143 153	0.000 228	3×10^{-4}	0.143 26	0.142 75
$5s$	0.089 196	0.089 065	0.000 131	2×10^{-4}	0.089 12	
$2p$	0.523 718	0.523 768	0.000 050	$4\times10^{-5*}$	0.523 79	0.5247
$3p$	0.229 798	0.229 582	0.000 216	2×10^{-4}	0.229 45	0.229 45
$4p$	0.128 255	0.128 134	0.000 121	1×10^{-4}	0.128 10	0.127 45
$5p$	0.081 687	0.081 610	0.000 077	7×10^{-5}	0.081 59	
$3d$	0.222 404	0.222 478	0.000 074	3×10^{-5}	0.222 45	0.222 35
$4d$	0.125 103	0.125 124	0.000 021	2×10^{-5}	0.125 14	0.124 85
$5d$	0.080 018	0.080 067	0.000 049	1×10^{-5}	0.080 08	
				Ne^{7+}			
$2s$	8.786 705	8.786 705	0.000 002			
$3s$	3.777 423	3.774 744	0.002 679	3×10^{-3}		
$4s$	2.091 777	2.090 726	0.001 051	1×10^{-3}		
$5s$	1.326 451	1.326 128	0.000 323	9×10^{-4}		
$2p$	8.214 384	8.202 803	0.011 581	$3\times10^{-4*}$		
$3p$	3.620 236	3.618 007	0.002 229	2×10^{-3}		
$4p$	2.027 378	2.025 570	0.001 808	1×10^{-3}		
$5p$	1.293 832	1.282 433	0.011 399	7×10^{-4}		
$3d$	3.559 267	3.558 774	0.000 493	8×10^{-4}		
$4d$	2.002 043	2.000 510	0.001 533	5×10^{-4}		
$5d$	1.280 18	1.280 155	0.000 025	3×10^{-4}		

our calculated energies and the experimental results is very small in all cases ($<5\times10^{-4}$ a.u.), and of the same order than those of Laughlin *et al.*[16] and Lin[17], which used more complicated model potentials. In particular, this difference is extremely small for the $1s^22p$ state, as discussed above. The largest difference with experimental data is found for the $n=3$ states, which is due to their slightly different exchange potential with respect to that of the $n=2$ electron (see Appendix A). In this respect, it should be noted that the use of a l-dependent model potential would not provide a better description for the Be^+ ion, since the main source of error is the variation in the exchange potential as a function of n. Although the $3d$ orbital presents the most different exchange potential (see Appendix A), its energy is in quite good agreement (as that of the $3s$ and $3p$) with the experimental one. This can be explained with the help of the first-order perturbation treatment of Appendix B, whose results are also given in Table II. It can be seen that this treatment reasonably predicts the order of magnitude of the small discrepancies between theory and experiment. Although the exchange potential differs from that of the $2s$ orbital for the largest values of n, its effect on the energies gets progressively smaller. In fact, these first-order corrections to the energies behave asymptotically as Eq. (19).

For the Ne^{7+} ion, the absolute differences with the experimental data are also small, although larger than for Be^+. The reason is that the slight difference between our V_m of Eq. (2) and the "real" potential $2V^d-V^{ex}$ gives corrections to the energy that increase like Z (Appendix B). In this system, a much larger energy difference is found for the $2p$ orbital than for Be^+. Moreover, while our perturbative treatment provides a good estimate for Be^+ (and also for Li and B^{2+}), it fails for more charged ions. This abnormally great energy difference for the $2p$

state can be only attributed to relativistic effects (in fact, they increase as Z^4 from C^{3+} to Mg^{9+}). For Ne^{7+}, the L-S splitting of the $2p$ state is about 0.2 eV. For more excited states, these relativistic effects are almost negligible.

It is also interesting to compare our results with those obtained with different model potentials for the Li atom, since it constitutes a benchmark for testing different model potential approaches and much work has been done on it. In Table III, we compare the energies of several ^2S, ^2P, and ^2D states of the Li atom [obtained with $\alpha=1.600365$ in Eq. (2) and the STO basis set of Table I] with some previous results found in the literature.[15,18−23] In spite of the simplicity of our model potential, we find similar or better agreement with the experimental results as that obtained with other—sometimes more elaborate—model (or pseudo) potentials. Only the results of Laughlin and Victor[22] are systematically better than ours, since they use a model potential that takes into account core polarization effects. Such effects are discussed in Sec. III.

III. TWO ELECTRONS IN THE FIELD OF A $1s^2$ CORE

A. The two-electron Hamiltonian

In Sec. II we have shown how a first-order approximation of the direct and exchange terms in Eqs. (7) and (8) leads to the simple form of the model potential V_m. This section is devoted to the study of the use of V_m for the case of two-active electrons in the field of a $1s^2$ core. Besides the interaction between the two-active electrons, the modification of the core effects due to the additional electron is a new feature of the problem.

The two-electron equation can be written in the general form[24,25]

TABLE III. Comparison between our energies (calculated with $\alpha=1.600365$ and the basis set of Table I) and other theoretical values for the $1s^2nl$ states of Li. The experimental data[15] are also included. All the values are referred to the $X^{(Z-2)+}(1s^2)$ core energy.

					$-E$ (a.u.)				
nl	Our results	Expt. (Ref. 15)	Ganas (Ref. 18)	Valance et al. (Ref. 19)	Goddard (Ref. 20)	Kahn and Goddard (Ref. 21)	Laughlin and Victor (Ref. 22)	Moore et al. (Ref. 23)
$2s$	0.198 14	0.198 14	0.1985	0.198 14	0.196 33	0.196 16	0.198 15	0.198 09
$3s$	0.074 35	0.074 18	0.0745	0.075 07	0.074 75	0.074 79	0.074 19	0.074 17
$4s$	0.038 70	0.038 62	0.0385	0.038 69	0.038 93	0.038 95	0.038 62	0.038 61
$5s$	0.023 69	0.023 64	0.0235	0.023 56	0.023 81	0.023 82	0.023 64	0.023 64
$6s$	0.015 97	0.015 94	0.0160		0.016 05	0.016 05	0.015 95	
$2p$	0.130 16	0.130 24	0.1305	0.130 23	0.112 33	0.128 75	0.130 20	0.130 05
$3p$	0.057 28	0.057 24	0.0575	0.057 80	0.051 07	0.056 85	0.057 23	0.057 17
$4p$	0.031 99	0.031 97	0.0320	0.032 21		0.031 82	0.031 98	0.031 95
$5p$	0.020 39	0.020 37	0.0205	0.020 49		0.020 30	0.020 38	0.020 36
$6p$	0.014 12	0.014 11	0.0140			0.014 05	0.014 11	
$3d$	0.055 58	0.055 61	0.0555	0.055 37	0.055 33	0.055 58	0.055 62	0.055 61
$4d$	0.031 26	0.031 27	0.0315	0.031 14		0.031 26	0.031 28	0.031 28
$5d$	0.020 01	0.020 01	0.0200	0.019 94		0.020 00	0.020 02	0.020 01
$6d$	0.013 89	0.013 90	0.0140			0.013 88		

$$\mathcal{H}_M(1,2) = H_m(1) + H_m(2) + V(1,2) , \tag{20}$$

where $H_m(i)$ has been defined in Eq. (12). The term $V(1,2)$ includes the interaction $1/r_{12}$ between the two-active electrons as well as additional "long-range" terms associated to polarization effects. If we retain only the two-pole polarization of the core, the polarization term has the form $V_{pol} \sim \alpha_d (r_1/r_1^3 + r_2/r_2^3)^2$. Due to the presence of the dielectric term $[r_1 r_2/(r_1^3 r_2^3)]$, the potential V_{pol} cannot be taken into account in our Feshbach approach (the same model potential must be used in the one-active and two-active electron cases). On the other hand, the terms of the form α_d/r_i^4 could be included in $V_m(r)$. In this work we neglect the polarization effects, such approximation is justified in our case for the following reasons.

(i) We are essentially interested in the case of heavy multicharged ions, and the polarization terms introduce two-order correction terms in the $1/Z$ energy expansion.

(ii) Only the long-range part of the wave functions will be affected; this should not affect the calculation of the widths whose values are determined by a "short-range operator" [in (28)—see below—$Q\mathcal{H}_M P$ reduces to $1/r_{12}$ in practice].

B. Theoretical approach for resonances and bound states

We have to solve the Schrödinger equation

$$[\mathcal{H}_M(1,2) - E]\chi^{L,S} = 0 , \tag{21}$$

where $\mathcal{H}_M$ is defined in (20) [with $V(1,2) = 1/r_{12}$] and L and S are, respectively, the total angular momentum and the total spin.

In II A we have noted the presence of a virtual state among the eigensolutions of Eq. (11). Due to the presence of this pseudoionization threshold, the resolution of Eq. (21) gives an infinite number of virtual states. The presence of such states is due to the model adopted here for the core $1s^2$ and has no physical signification. It has been pointed out[26,27] that the calculation of bound states is formally equivalent to the problem of the determination of doubly excited states. Indeed, the bound states and resonances lie above one or more ionization thresholds (for bound states it is a virtual one). As a consequence the bound states are embedded in a pseudocontinuum and they may be treated formally as resonances. The method adopted here is similar to the Feshbach approach applied by Bachau[28] for the two-electron case. We introduce the projection operators P and Q defined by

$$Q = 1 - P , \tag{22}$$

where

$$P = P_1 + P_2 - P_1 P_2 \tag{23}$$

$$\text{and } P_i = \sum_{n=1}^{N-1} \sum_{l=0}^{n-1} \sum_{m=-l}^{l} |\phi_{nlm}(i)\rangle\langle\phi_{nlm}(i)| . \tag{24}$$

N specifies the threshold above the series of bound or autoionizing states considered, and $\phi_{nlm}(i)$ is a one-electron orbital [Eq. (11)] associated to each (real or virtual) ionization threshold. Therefore, for bound states the sum-

mation is limited to the virtual $\phi_{1s}(i)$ states; for autoionizing states one must include all the threshold states whose energies lie below that of the N threshold. For example, for the $1s^2 3ln'l'$ series, the operator P includes the ϕ_{1s}, ϕ_{2s}, and ϕ_{2p} wave functions. Then the unshifted energy of the states under consideration is obtained through the resolution of the equation

$$(Q\mathcal{H}_M Q - E_s)\chi_s^{L,S} = 0 . \tag{25}$$

The function $\chi_s^{L,S}$ is expanded on a set of configurations of a given symmetry:

$$\chi_s^{L,S} = \sum_n a_{ns} U_n^{L,S} \tag{26}$$

with

$$U_n^{L,S} = \mathcal{A} \bar{\phi}_{n_1 l_1}(1)\bar{\phi}_{n_2 l_2}(2)\mathcal{Y}_{l_1,l_2}^{L,M}(1,2) , \tag{27}$$

where $\mathcal{A}$ is the antisymmetrization operator, $\bar{\phi}_{nl}(i)$ is the radial part of the wave function $\phi_{nl}(i)$ defined in Eq. (11), and $\mathcal{Y}_{l_1,l_2}^{L,M}(1,2)$ is the usual angular part.

The coefficients a_{ns} are determined through diagonalization of Eq. (25) in the representation of the $U_n^{L,S}$ basis. At this point it is worth recalling that our definition of the operator P is consistent with the first-order approximation (see III A) where both electrons "see" the same model potential V_m. Then, in our calculation, all terms of first order in a $1/Z$ expansion are consistently included.

For resonant states, we briefly recall the golden-rule-like expression for partial widths:

$$\Gamma_{\beta,\gamma} = 2\pi |\langle \chi_s^{L,S}|Q\mathcal{H}_M P|\chi^{\beta,\gamma}\rangle|^2 . \tag{28}$$

$\chi^{\beta,\gamma}$ is a nonresonant function of the continuum, β is the final state of the ion $(2s,2p,3s,3p,3d,\dots)$, and γ represents the orbital quantum number of the ejected electron $(\epsilon s, \epsilon p, \dots)$. $\chi^{\beta,\gamma}$ is obtained in the static exchange approximation through a discretization procedure (see Ref. 8 and references therein) by solving

$$(P\mathcal{H}_M P - E)\chi^{\beta,\gamma} = 0 \tag{29}$$

with $E = E_s$. After diagonalization of $P\mathcal{H}_M P$ for each (β,γ) channel in an appropriate $L2$ basis set (Ref. 8), the total width Γ is given by

$$\Gamma = \sum_{\beta,\gamma} \Gamma_{\beta,\gamma} . \tag{30}$$

C. Calculations

For illustration we have chosen the Be and Ne^{6+} systems. We have solved the secular equation corresponding to the model Hamiltonian of Eq. (25) in a basis of configurations built from the basis set of Slater-type orbitals given in Table I. The values of the parameter α are the same of those given in Sec. II (2.333 710 and 6.366 365, respectively) which were chosen to exactly reproduce the experimental $^2S(1s^2 2s)$ ground-state energy. In Table IV we present our results for several bound and resonant states for both systems, compared with oth-

er experimental[15] and theoretical data.[17,29,30,22] For the bound states of Be given in this table ($2s^2, 2s3s, 2s4s, 2s2p, 2s3p$), the agreement with the experimental data is very good. The differences ($\sim 10^{-3}$ a.u.) are comparable to those given in Table II for the $1s^2nl$ states.

The $^1S^e(1s^22p^2)$ state of Be was considered for a long time as a bound state (see for example Refs. 15, 31, and 32). However, recent experiments[33-35] and calculations[17,29,30,36,22] have shown that it is a resonant state. In this case our Feshbach calculations (which include the ϕ_{1s} and ϕ_{2s} orbitals in P—[see Eq. (24)]) give an unshifted energy which lies below the $2s$ ionization threshold. Due to the closeness of the $2s$ and $2p$ ionization thresholds one can expect that the Feshbach approach is inadequate to calculate the position of the $^1S^e(1s^22p^2)$ state; in other words the shift should be calculated. Therefore, we have used a stabilization procedure [where the $2sns$

configurations are included, that is, only the ϕ_{1s} orbital is included in Eq. (24)]. The positions of the $^1S^e(1s^22p^2)$ state is that given in Table IV ($-0.655\,08$ a.u.) and it lies above the ionization threshold $1s^22s$. This confirms that the $^1S^e(1s^22p^2)$ state is resonant and presents strong contributions of the $2sns$ configurations, as pointed out by Norcross and Seaton.[30] Our results also show that the energies of the $1s^22pnp$ and $1s^22pnd$ states with $n > 2$ lie above the $1s^22s$ ionization threshold of Be. Unfortunately, few accurate experimental values are available and then our comparison is carried out with other theoretical calculations. For the $1s^22pnp$ and $1s^22pnd$ states with $n > 2$, the general agreement is very good (the discrepancies are of the same order than for bound states). Our result for the $1s^22p^2$ state agrees very well with two of the four previous theoretical calculations.[22,30] For the Ne^{6+} ion, all the $1s^22pnp$ and $1s^22pnd$ states are bound. The agreement of our results with the experimental data leads

TABLE IV. Energies for some $^1S^e$ and $^1P^o$ $1s^22lnl'$ bound and resonant states of (a) Be and (b) Ne^{6+}, obtained with $\alpha = 2.333\,710$ and $\alpha = 6.366\,365$, respectively, the basis set of Table I, and all possible $\phi_{nl}\phi_{n'l'}$ configurations with $n,n' \leq 5$ [see Eq. (27)]. Comparison between our results and other theoretical and experimental[15] data. All the values are referred to the $X^{(Z-2)+}(1s^2)$ core energy.

			$-E$ (a.u.)			
			Laughlin and	Norcross and	Moccia[a] and	
	This	Expt.	Victor	Seaton	Spizzo	Lin
$2lnl'$	work	(Ref. 15)	(Ref. 22)	(Ref. 30)	(Ref. 29)	(Ref. 17)
			(a) Be			
$^1S^e\ 2s^2$	1.007 43	1.011 85	1.009 25	1.0111		1.008 55
$2s3s$	0.761 19	0.762 72	0.7618	0.7625	0.763 43	0.757 45
$2s4s$	0.713 92	0.714 57	0.7142		0.715 43	0.711 95
Threshold	0.669 25	0.669 25				
$2p^2$	0.655 08	0.6647[b]	0.6551	0.657 20	0.662 27	0.6598
$2p3p$	0.577 13				0.577 58	0.577 85
$^1P^o\ 2s2p$	0.810 06	0.817 90	0.8105	0.8154	0.817 89	0.8061
$2s3p$	0.734 92	0.737 61	0.7335	0.7370	0.738 25	0.726 55
$2s4p$	0.704 37		0.7054		0.707 16	0.7012
Threshold	0.669 25	0.669 25				
$2p3s$	0.639 98		0.616 05	0.6088		0.6264
$2p4s$	0.589 91		0.566 25			0.571 15
$2p3d$	0.575 50	0.5759[b]	0.5745		0.573 57	0.5761
$2p5s$	0.561 23					
$2p4d$	0.549 20		0.551 35		0.551 17	0.5538
			(b) Ne^{6+}			
$^1S^e\ 2s^2$	16.3955	16.4039				
$2p^2$	14.5944	14.6024				
$2s3s$	11.8459	11.8555				
$2s4s$	10.4314	10.4511				
$^1P^o\ 2s2p$	15.4064	15.4245				
$2s3p$	11.7284	11.7306				
$2p3s$	11.2096	11.1944				
$2p3d$	10.8471	10.8581				

[a]All energies reported by these authors are referred to the $1s^22s^2$ ground-state energy. In order to compare with other results we have shifted their values according to the experimental $1s^22s^2$ energy.
[b]Experimental values of Clark *et al.* (Ref. 35). They have been shifted according to the experimental energies of the $1s^22s^2$ and $1s^22s$ states given here.

TABLE V. Energies, partial widths, and total widths of the $1s^2 4l4l'$ $^1S^e$ and $^1P^o$ resonant states of N^{3+} and Ne^{6+} obtained with $\alpha=4.402\,872$ and $\alpha=6.366\,365$, respectively, and the basis set given in Table VI. All possible $\phi_{nl}\phi_{n'l'}$ configurations with $4 \leq n,n' \leq 8$ are built. All the values are referred to the $X^{(Z-2)+}(1s^2)$ core energy. $[-x]$ denotes $\times 10^{-x}$.

$-E$ (a.u.)	Γ (eV)	$\Gamma_{2s\epsilon s}$	$\Gamma_{2p\epsilon p}$	$\Gamma_{3s\epsilon s}$	$\Gamma_{3p\epsilon p}$	$\Gamma_{3d\epsilon d}$
			N^{3+} $^1S^e$			
1.5128	0.576[-1]	0.552[-2]	0.107[-2]	0.509[-1]		
1.4153	0.2227	0.482[-2]	0.367[-1]	0.318[-1]	0.1493	
1.3385	0.5511	0.218[-5]	0.203[-3]	0.362[-1]	0.1159	0.3987
1.2362	0.438[-1]	0.524[-2]	0.894[-3]	0.325[-1]	0.514[-2]	0.849[-5]
			Ne^{6+} $^1S^e$			
3.9323	0.765[-2]	0.690[-2]	0.747[-3]			
3.7637	0.896[-1]	0.486[-2]	0.452[-1]	0.395[-1]		
3.6278	0.384[-1]	0.208[-4]	0.111[-3]	0.382[-1]		
3.4134	0.194[-2]	0.181[-3]	0.353[-3]	0.183[-4]	0.132[-2]	0.584[-4]

$-E$ (a.u.)	Γ (eV)	$\Gamma_{2s\epsilon p}$	$\Gamma_{2p\epsilon s}$	$\Gamma_{2p\epsilon d}$	$\Gamma_{3s\epsilon p}$	$\Gamma_{3p\epsilon s}$	$\Gamma_{3p\epsilon d}$	$\Gamma_{3d\epsilon p}$	$\Gamma_{3d\epsilon f}$
				N^{3+} $^1P^o$					
1.4541	0.652[-1]	0.899[-2]	0.156[-1]	0.401[-2]	0.365[-1]				
1.3763	0.5023	0.116[-4]	0.893[-3]	0.227[-2]	0.519[-1]	0.582[-1]	0.1003	0.2072	0.815[-1]
1.2665	0.889[-1]	0.153[-3]	0.358[-4]	0.274[-2]	0.101[-2]	0.147[-5]	0.135[-1]	0.142[-2]	0.701[-1]
				Ne^{6+} $^1P^o$					
3.8327	0.333[-1]	0.104[-1]	0.175[-1]	0.531[-2]					
3.6947	0.692[-1]	0.292[-4]	0.125[-2]	0.403[-2]	0.639[-1]				
3.4955	0.1119	0.318[-3]	0.434[-4]	0.351[-2]	0.138[-2]	0.283[-3]	0.206[-1]	0.103[-2]	0.846[-1]

to the same conclusions as for Be. In this case, the discrepancies are greater than for Be ($\lesssim 0.01$ a.u.) and we have tested that they increase linearly with Z. As we have mentioned above this is due to the fact that Eq. (15) is not exactly verified since a very small contribution of the exchange potential is neglected.

Very recently Boudjema et al.[37] have compared (using a fitting procedure) the $A^{(Z-4)+}(1s^2 3l3l')$ lines observed in $A^{(Z-2)+}(1s^2)+$He collisions ($Z=7$, 8, and 10). A very nice fit of the observed lines is obtained with the theoretical values calculated through our procedure. We have made calculations for the $A^{(Z-4)+}(1s^2 3ln'l')$ states with $Z=4-10$ and $n'=3,4$. We have considered $^{1,3}S^e$, $^{1,3}P^{e,o}$, $^{1,3}D^{e,o}$, $^{1,3}F^{e,o}$, and $^{1,3}G^{e,o}$ symmetries. The partial widths associated with the $A^{(Z-3)+}(1s^2 2s)$ and $A^{(Z-3)+}(1s^2 2p)$ final states have been also calculated, as well as information about the structure of the states. Presentation of this amount of data is out of the scope of the present publication and has been reported elsewhere.[38]

We have extended these calculations to the $1s^2 4l4l'$ doubly excited states. This case has a special interest since, depending on the nuclear charge, some of these resonances lie above or below the $1s^2 3l$ ionization limits (this has been observed experimentally by Bordenave-Montesquieu et al.[39] for the N^{5+}). As a consequence there are strong variations of the widths in the isoelectronic series. In Table V we present energy positions, partial widths, and total widths for the $^1S^e$ and $^1P^o$ $1s^2 4l4l'$ resonant states of N^{3+} and Ne^{6+} calculated with the basis set shown in Table VI. These have been obtained

with a P operator which includes the ϕ_{1s}, ϕ_{2s}, ϕ_{2p}, ϕ_{3s}, ϕ_{3p}, and ϕ_{3d} solutions of (11). In this case the $n=3$ and $n=4$ thresholds are well separated in energy, which justifies our P-Q partitioning. The variation of the widths for N^{3+} and Ne^{6+} mentioned above is clearly illustrated in Table V. For example, the lowest $^1S^e$ state of N^{3+} lies above the $1s^2 3s$ ionization threshold whereas it is below such threshold for Ne^{6+}. As a consequence there is a large difference between the widths of this state in the two cases. The numerical accuracy of the results has been checked by varying the basis sets (for open and closed channels). As an example we show in Table VII the parameters obtained for the two lowest $^1S^e$ states of $N^{3+}(4l4l')$, using different basis sets for the closed chan-

TABLE VI. STO basis set used in the calculation of energies in Table V. See the definition of each STO in Table I, here $\zeta_i = 1/N$.

N	$l=0$	$l=1$	$l=2$	n $l=3$	$l=4$	$l=5$	$l=6$
1	1						
2	1–2	2					
3	1–3	2–3	3				
4	4–6	4–6	3–4	4			
5			5–6	4–5	5		
6				6–7	5–6	6	
7	7–9	7–9	7–9		7	6–7	7
8							8

TABLE VII. Energies, partial widths, and total widths of the two lowest $1s^2 4l4l'$ $^1S^e$ resonant states of N^{3+} calculated with different basis sets. The configurations $\phi_{nl}\phi_{n'l'}$ used are shown in the table. $[-x]$ denotes $\times 10^{-x}$.

$-E$ (a.u.)	Γ (eV)	$\Gamma_{2s\epsilon s}$	$\Gamma_{2p\epsilon p}$	$\Gamma_{3s\epsilon s}$	$\Gamma_{3p\epsilon p}$
		$4 \leq n, n' \leq 7$			
1.5127	0.588([−1]	0.579[−2]	0.115[−2]	0.519[−1]	
1.4147	0.233	0.497[−2]	0.383[−1]	0.328[−1]	0.157
		$4 \leq n, n' \leq 8$			
1.5128	0.576[(−1]	0.552[−2]	0.107[−2]	0.509[−1]	
1.4153	0.223	0.482[−2]	0.367[−1]	0.318[−1]	0.149

nels. We note the good stability of the energies and widths, in the case of partial width the relative differences do not exceed 10%. A systematic study of all the series is in progress.

IV. CONCLUSIONS

We have studied the use of the model potential of Eq. (2) for nonrelativistic one-and two-electron systems in the field of a $1s^2$ core and the approximations involved in using this form. We have shown that for $1s^2 nl$ states the model potential of Eq. (2) can account to a good approximation for the direct and (nonlocal) exchange potentials of the outer electron with the core. We have quantitatively explained why this can be achieved by simply fitting its α parameter to reproduce the exact $^2S(1s^2 2s)$ ground-state energy. In this way, good agreement with the experimental energies is also found for the excited states, almost independently of l. In this respect, we have shown that the exchange potential between a $2p$ electron and the core is very similar, up to first order, as that of a $2s$ electron for small r and that the progressive difference in exchange potentials for more excited states barely affects their energy positions.

For two electrons in the field of the $1s^2$ core ($1s^2 nln'l'$ states), we have shown that the model potential of Eq. (2) with the α value fitted to the $1s^2 2s$ energy is still valid. This has been illustrated by our calculations of the energies of bound and resonant states of Be and Ne^{6+}.

Our one-parameter model potential provides energy results for $1s^2 3l3l'$ resonant states which has permitted, for the first time, a correct interpretation of experimental results.[37] One must note that the resolution of such experimental spectrum requires the calculations of the positions and partial widths. In this case, the accuracy is of the same order of magnitude as the typical average experimental error, so that the use of this model potential approach can provide theoretical results that help to interprete electron spectra and analyze the structure and characteristics of the resonant states. In this paper we have given new results for the energies and widths of the $1s^2 4l4l'$ $^1S^e$ and $^1P^o$ states of N^{3+} and Ne^{6+}.

The advantage of our approach is that it leads to a two-electron problem and the extension of the Feshbach techniques for the calculation of resonant states can be carried out in a simple way. This is particularly remarkable since the implementation of the Feshbach method

for three- or four-electron systems is a cumbersome task.[40,41] It must be stressed that our treatment of the two-valence electrons in the presence of the $1s^2$ core goes beyond a simple Hartree-Fock approach because a direct configuration-interaction calculation is performed. Similar quantitative conclusions for excited two-valence-electron states in the field of more complicated closed-shell cores are not guaranteed by our present study and a further analysis would be necessary.

APPENDIX A: FIRST-ORDER CALCULATION OF THE EXCHANGE POTENTIAL OF AN ELECTRON WITH A $1s^2$ CORE IN THE LIMIT $r=0$

The exchange potential for one electron in a ϕ_{nl} orbital, which is in the field of a $1s^2$ core, is defined [see Eqs. (13) and (14)]:

$$V_{nl}^{ex}(r_1) \equiv \frac{V^{ex}(r_1)\phi_{nl}(r_1)}{\phi_{nl}(r_1)}$$

$$= \frac{\left[\int \phi_{1s}(r_2)r_{12}^{-1}\phi_{nl}(r_2)dr_2\right]\phi_{1s}(r_1)}{\phi_{nl}(r_1)} . \quad (A1)$$

Using hydrogenic orbitals to describe the ϕ_{nl} orbitals and the expansion of r_{12}^{-1} in spherical harmonics, integrating over the angular coordinates leads to the equation

$$V_{nl}^{ex}(r_1) = \frac{R_{10}(r_1)}{(2l+1)R_{nl}(r_1)} \int_0^\infty R_{10}(r_2)R_{nl}(r_2)$$

$$\times \frac{r_<^l}{r_<^{l+1}}r_2^2\,dr_2 , \quad (A2)$$

where R_{nl} are the radial hydrogenic functions. It may be easily shown that

$$V_{nl}^{ex}(r=0)=\frac{4Z}{2l+1}(n-l-1)!(2l+1)!\sum_{k=0}^{n-l-1}\frac{(-1)^k(k+1)2^kn^2}{(n-l-1-k)!(2l+1+k)!(n+1)^{k+2}} .$$ (A3)

For the $n=2$ and $n=3$ cases, this equation gives

$$V_{2s}^{ex}(r=0)=V_{2p}^{ex}(r=0)=\tfrac{16}{27}Z\simeq0.5926Z ,$$ (A4)

$$V_{3s}^{ex}(r=0)=V_{3p}^{ex}(r=0)=\tfrac{9}{16}Z\simeq0.5625Z ,$$ (A5)

$$V_{3d}^{ex}(r=0)=\tfrac{9}{20}Z=0.45Z .$$ (A6)

The difference between V_{2s}^{ex} and V_{2p}^{ex} comes from the first-order term in r. Indeed, Eqs. (13) and (14) lead to

$$V_{2s}^{ex}(r)\underset{r\to0}{\sim}\tfrac{16}{27}Z+ZO(Zr^2) ,$$ (A7)

$$V_{2p}^{ex}(r)\underset{r\to0}{\sim}\tfrac{16}{27}Z-\tfrac{8}{27}Z^2r+ZO(Zr^2)$$ (A8)

(notice that V_{2s}^{ex} has no term in r since it presents a maximum at $r=0$, see Fig. 2).

APPENDIX B: A PERTURBATION APPROACH TO ESTIMATE THE ERROR IN THE ENERGY OF A $1s^2nl$ STATE

In the previous Appendix we have shown that the exchange potential between an outer electron and two $1s$ core electrons depends on n and l. Then, different model potentials should be used for different values of n and l. However, in practice, one uses the same model potential of Eq. (2)—with a value of α, which gives the $1s^22s$ ground-state energy—to obtain all the states. Thus, the error in the potential for the nl excited states can be written

$$V_p=2(\alpha_{2s}e^{-2\alpha_{2s}r}-\alpha_{nl}e^{-2\alpha_{nl}r})+2r^{-1}(e^{-2\alpha_{2s}r}-e^{-2\alpha_{nl}r}) ,$$ (B1)

where α_{2s} and α_{nl} are the values associated to the energies of the ground $2s$ and excited nl states, respectively. In a first-order approximation, the corrections to the energies of the excited states will be

$$E_{nl}^{(1)}=\langle\phi_{nl}|V_p|\phi_{nl}\rangle ,$$ (B2)

where V_p is given by (B1). Since we are only interested in obtaining an estimation of this correction, we can use, for α_{2s} and α_{nl}, the exchange potentials in $r=0$ calculated in Appendix A. Then we find

$$\alpha_{nl}=Z-\frac{2Z}{2l+1}(n-l-1)!(2l+1)!\sum_{k=0}^{n-l-1}\frac{(-1)^k(k+1)n^22^k}{(n-l-1-k)!(2l+1+k)!(n+1)^{k+2}} .$$ (B3)

Using Eqs. (B3) and (B1) and hydrogenic orbitals with $Z_e=Z-2$ in Eq. (B2), $E_{nl}^{(1)}$ can be easily calculated. The results are given in Table II.

To find the energy error in the $2p$ orbital, we must use the more elaborate exchange potential of (A8) since $V_{2p}^{ex}=V_{2s}^{ex}$ at $r=0$. Using hydrogenic orbitals with $Z_e=Z-2$, the mean value $\langle\Delta V_{2p}^{ex}\rangle$, of the r-dependent part of $V_{2p}^{ex}(r)$ [Eq. (A8)] in the core region will be given approximately by

$$\langle\Delta V_{2p}^{ex}\rangle\equiv\int_0^{1/Z_e}R_{2p}^2(r)(-\tfrac{8}{27}Z^2r)r^2dr$$

$$=\frac{1}{3}\left[\frac{Z_e}{2}\right]^3Z_e^2\int_0^{1/Z_e}e^{-Z_er}r^4(-\tfrac{8}{27}Z^2r)dr .$$ (B4)

The integration of Eq. (B4) leads to

$$\langle\Delta V_{2p}^{ex}\rangle=-\frac{8}{27}\frac{Z^2}{Z_e}(-\tfrac{163}{12}e^{-1}+5) .$$ (B5)

This expression accounts for the very slight difference shown in Fig. 2 between the empirical V_m potential and our theoretical one $2V^d-V_{2p}^{ex}$ in the core region. Then, a more precise value of α_{2p} will be

$$2\alpha_{2p}=2Z-\frac{16}{27}Z+\frac{8}{27}\frac{Z^2}{Z_e}(\tfrac{163}{12}e^{-1}+5) .$$ (B6)

For the $2p$ orbitals of Table II, we have used this expression in Eq. (B1) to estimate $E_{2p}^{(1)}$ in Eq. (B2).

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