Correlated expansions of $n\,^1S$ and $n\,^3S$ states for two-electron atoms in exponential cosine screened potentials

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(Received 4 October 2013; published 15 January 2014)

Two–electron atoms embedded in a plasma environment are studied with screened and exponential cosine screened Coulomb model potentials. Within a configuration interaction approach, and using parameter–free explicitly correlated basis functions, we have calculated the ground-state and first excited-state energies (and other mean values) for H^-, He, and Li^+. We analyze their evolution with the screening parameter and provide simple fits, which allow for practical and rapid evaluations for example in plasma applications.

DOI: 10.1103/PhysRevA.89.012507 PACS number(s): 32.30.−r, 31.15.ve, 31.15.vj

I. INTRODUCTION

The bound states of three-body atomic or molecular systems are usually calculated assuming the three particles interact through Coulomb potentials. While this is correct for systems placed in a vacuum, when they are placed in an external environment the potentials change; according to the environment the interactions can be described by model potentials. As a result the energy levels and other properties of the considered system change considerably. It is the purpose of this paper to investigate how this occurs in screened potentials for two-electron atoms and ions.

For a quantum plasma environment, a general model potential between two particles of charges z_i and z_j at a distance r reads, in atomic units,

$$U(r) = z_i z_j \frac{e^{-\lambda r}}{r} \cos(\delta r), \tag{1}$$

where λ and δ are positive real parameters. The potential (1) is written in a general way to include various subcases:

$\lambda = \delta = 0$ (case A). This case corresponds to the usual Coulomb (C) potential which applies in the vacuum.

$\delta = 0$ (case B). In a weakly coupled plasma the interaction can be described by the Debye-Hückel model or screened Coulomb potential (SCP), which corresponds to $\delta = 0$ (see, e.g., Refs. [1–4] and references therein). The parameter λ, known as the screening parameter, is related to the plasma frequency ω_P and the thermal velocity v_T through $\lambda = \omega_P/v_T = \sqrt{4\pi e^2 N_e/(k_B T_e)}$, where k_B is the Boltzmann constant, and N_e and T_e are the plasma-electron density and temperature, respectively. Alternatively, one may use the Debye screening length D, with $\lambda = 1/D$.

$\lambda = \delta \neq 0$ (case C). When the plasma density increases, multiparticle cooperative interactions modify the picture and the Debye-Hückel model is not reliable anymore [5]. In Ref. [6] (see also [7]), Shukla and Eliasson have shown that for dense quantum plasmas the effective potential can be modeled by a modified Debye-Hückel potential or exponential cosine screened Coulomb potential (ECSCP), which is given by Eq. (1) with $\delta = \lambda \neq 0$. Again, the screening parameter λ is related to the electron plasma frequency, though in a different manner: according to Ref. [6], $\lambda = k_q/\sqrt{2} = \sqrt{m_e \omega_P/\hbar}$, where k_q is the quantum wave number, and is independent of the charge velocity. The screening effect is stronger than in SCP because of the presence of the oscillatory cosine factor. Hence the atomic properties in a dense quantum plasma will be different from those in a weakly coupled plasma. The ECSCP potential differs in shape from the Debye-Hückel one since it presents, for $z_i z_j > 0$, a minimum (at $r \simeq 3/k_q$) similarly to the Lennard-Jones potential for atoms. With different significance of λ for each case, ECSCP models are used also in other branches of physics, with applications in diverse fields such as astrophysics, nuclear, or solid-state physics (see Introduction of Ref. [8]). For, example, the interaction (1) models the potential between an ionized impurity and an electron in metal, and the ionized impurity-electron potential in a semiconductor.

According to the plasma density, in a plasma environment the three interactions of a two-electron atom may by modeled with SCP or ECSCP. For the SCP case, ground and excited states have been studied for some time and in some detail (see, for example, Refs. [9–13] and several older references cited therein). On the other hand, for ECSCP much less has been presented in the literature. In very recent papers Ghoshal and Ho [8,14] have published the first calculations of the ground states of H^- and He in an ECSCP on a wide range of screening parameters λ. Highly correlated Hylleraas-type expansions with 252 up to 525 terms were used to evaluate the energy as a function of λ . For H^-, mean values $\langle r_{ij}^p \rangle$, with $p \in \mathbb{Z}$, were also provided. While the same authors also studied doubly excited-state resonance states for both H^- [14] and He [15], the $n\,^{1,3}S$ excited states of He were not investigated. Also, we look at two-electron positive ions in this model; in view of their interest, for example, in plasma applications, we believe it is worth extending the study to ionized species.

This paper is concerned with two-electron atoms in ECSCP and has several aims. One is to confirm the published results with relatively simpler wave functions using a correlated basis, which has proved quite efficient for a wide range of three-body systems [16-19]. The main aim is to extend the findings in various directions: (i) we include also the Li^+ ion to observe the expected evolution with the nuclear charge z_3; (ii) we evaluate the mean values $\langle r_{ij}^p \rangle$ also for He and Li^+; (iii) we provide analytical fits of the energy $E(\lambda)$ and some mean values $\langle r_{ij}^p \rangle(\lambda)$ for both SCP and ECSCP models, i.e., an easy to use tool to estimate the evolution of these quantities with the screening parameter λ; (iv) we make a systematic

investigation of the critical value λ_c value for which the ground state ceases to exist, i.e., $E(\lambda_c) = 0$, and provide a simple predictive tool for any z_3 by extending the investigation further into the isoelectronic series (this may be of interest for plasma applications); and (v) we also analyze the evolution with λ of the energy spectrum, by providing the energies of the first four simply S excited states of He and Li^+ with SCP and ECSCP (most of these energy levels are presently not available in the literature).

Our calculations are performed with a configuration interaction approach with non-linear parameter-free correlated basis functions which explicitly depend on the three interparticle distances. Named C3-like, it has been presented before [16,20] and applied for the study of ground and excited states of a number of three-body systems [17–19]. Each basis function is analytical and parameter free; it consists of the product of two hydrogenic functions multiplied by a distortion factor such that it overall satisfies exactly all three two-body Kato cusp conditions [21]. Further correlation is introduced through a multiplying polynomial as proposed in [23,24]. Consequently, the constructed trial wave functions involve only linear parameters which are obtained through a single diagonalization. As we have opted to use a limited number of such parameters, our trial wave functions do not aim to compete with highly accurate proposals previously published, but rather to provide a multitude of results which may be used, as illustrated in this contribution, to construct simple and practical fits in term of the screening parameter λ.

The rest of the paper is arranged as follows. In Sec. II we briefly describe the theoretical framework and the basis set be used. In Sec. III we present our results for both ground and excited states for three two-electron systems with SCP and ECSCP. Energies and other expectation values are compared to previously published values, when available, and practical fits are provided as a function of the screening parameter. Finally a summary is given in Sec. IV.

Hartree atomic units ($\hbar = m_e = e = 1$) are used throughout this paper.

II. THEORY

Consider atomic systems composed of three particles with charges $z_1 < 0$, $z_2 < 0$, $z_3 > 0$, and respective masses m_1, m_2, m_3. Let $\mu_{ij} = \frac{m_i m_j}{m_i + m_j}$ $(i \neq j)$ be the reduced masses. We shall designate as particle 3 the heaviest particle, i.e., the nucleus of mass m_3 and charge z_3, and the two lighter particles, labeled 1 and 2, with masses m_1,m_2 and charges $z_1 = z_2 = -1$. The vectors $\mathbf{r}_{13}$ and $\mathbf{r}_{23}$ will denote the two lighter particles' positions with respect to the nucleus, and $\mathbf{r}_{12} = \mathbf{r}_2 - \mathbf{r}_1$ their relative position.

As we consider here only S states, we may use the interparticle (Hylleraas) coordinates (r_{13}, r_{23}, r_{12}). For the general charges z_1, z_2, and z_3, the six-dimensional Schrödinger equation reduces to the following Hylleraas equation

$$H\Psi(r_{13},r_{23},r_{12}) = E\Psi(r_{13},r_{23},r_{12}), \tag{2}$$

where the nonrelativistic Hamiltonian H is given by

$$H = D_0 + D_1 \tag{3}$$

with

$$D_0 = \sum_{i,j=1,2,3,j>i} \left[-\frac{1}{2\mu_{ij}} \left(\frac{\partial^2}{\partial r_{ij}^2} + \frac{2}{r_{ij}} \frac{\partial}{\partial r_{ij}} \right) + U_{ij}(r_{ij}) \right], \tag{4}$$

$$D_1 = \sum_{i,j,k=1,2,3,j\neq i,j\neq k,k>j} \left[-\frac{1}{m_i} \frac{r_{ik}^2 - r_{jk}^2 + r_{ij}^2}{2r_{ik}r_{ij}} \frac{\partial^2}{\partial r_{ik}\partial r_{ij}} \right], \tag{5}$$

and where the potentials $U_{ij}(r_{ij})$ are given by Eq. (1) with parameters λ_{ij} and δ_{ij}. The three singularities ($r_{ij} = 0$) of such ECSCP or SCP potentials are the same as in the Coulomb case for whatever parameter values λ_{ij} and δ_{ij}: the solution should therefore satisfy the three two-body Coulomb cusp conditions, known as Kato cusp conditions [21]. Above, no assumptions are made that some parts of the Hamiltonian are negligible in comparison to others. The operator D_1 contains no singularities, and is nondiagonal as it mixes the three relative coordinates. When the nucleus is (virtually) considered as infinitely heavy ($m_3 \to \infty$), the term $i = 3$ in D_1 is absent. Such limit is often taken as reference system.

To build an approximate solution we propose a combination of functions written as

$$\psi^{(N_1,N_2,N_3)}_{n_1,n_2,n_3}(r_{13},r_{23},r_{12}) = \phi^{C3}_{n_1,n_2,n_3}(r_{13},r_{23},r_{12}) \times \Omega^{(N_1,N_2,N_3)}_{n_1,n_2,n_3}(r_{13},r_{23},r_{12}), \tag{6}$$

where n_1,n_2,n_3,N_1,N_2,N_3 are positive integers. In Refs. [20] and [16], one of the present authors proposed a basis set, labeled C3, that solves exactly the diagonal D_0 part of the three-body Schrödinger Eq. (2) in the case of pure Coulomb potentials. Defining the quantities $k_{i3} = \frac{z_i z_3 \mu_{i3}}{n_i} = -\sqrt{-2\mu_{i3}E_{i3}} < 0$, where E_{i3} are the energies associated to the pairs $(i,3)$, the basis functions are given by

$$\phi^{C3}_{n_1,n_2,n_3}(r_{13},r_{23},r_{12}) = \varphi_{n_1}(r_{13})\,\varphi_{n_2}(r_{23})\,{}_1F_1\left(-n_3,2,-2\frac{z_1 z_2 \mu_{12}}{n_3} r_{12}\right), \tag{7}$$

where

$$\varphi_{n_i}(r_{i3}) = \sqrt{\frac{1}{2}}\,(-2k_{i3})^{3/2} \times e^{k_{i3}r_{i3}}\,{}_1F_1\,(1-n_i,2,-2k_{i3}r_{i3}) \quad i = 1,2 \tag{8}$$

are normalized hydrogenic functions with principal quantum numbers n_i and zero angular momenta [22], and the distortion factor ${}_1F_1\,(-n_3,2,-2z_1z_2\mu_{12}r_{12}/n_3)$ reduces to a Laguerre polynomial $L^{(1)}_{n_3}(-2z_1z_2\mu_{12}r_{12}/n_3)$. Each basis function $\phi^{C3}_{n_1,n_2,n_3}(r_{13},r_{23},r_{12})$, is explicitly correlated, and satisfies exactly the two-body Kato cusp conditions [21], but do not include appropriate information about the asymptotic conditions. For a given set of quantum numbers $\{n_1,n_2,n_3\}$—one for each coordinate—the basis functions are parameter free.

As indicated by Eq. (6), for each set $\{n_1,n_2,n_3\}$ we introduce further correlation which, according to what is suggested in

Refs. [23,24], reads

$$\Omega^{(N_1,N_2,N_3)}_{n_1,n_2,n_3}(r_{13},r_{23},r_{12}) = \sum_{i,j,k\neq 1}^{N_1,N_2,N_3} c^{n_1n_2n_3}_{ijk} r^i_{13} r^j_{23} r^k_{12}, \qquad (9)$$

where N_1, N_2, and N_3 represent the number of linear coefficients included for each of the relative coordinates. For two identical light particles (as for two-electron atoms) the linear parameters are such that $c^{n_1n_2n_3}_{ijk} = c^{n_1n_2n_3}_{jik}$ by symmetry. In order to have the trial wave functions (6) satisfying the Kato cusp conditions, the coefficients $c^{n_1n_2n_3}_{ijk}$ corresponding to first powers in coordinates should not appear. The polynomials $\Omega^{(N_1,N_2,N_{k3})}_{n_1,n_2,n_3}$ add extra correlation to the function of Eq. (6), in addition to that already included in the basis functions $\phi^{C3}_{n_1,n_2,n_3}$.

In the case of S states, the angularly correlated configuration interaction method constructs an approximate solution of the Hylleraas equation (2) as a linear combination of the basis functions (6)

$$\Psi_M = N \sum_{n_1,n_2,n_3} \psi^{(N_1,N_2,N_3)}_{n_1,n_2,n_3}(r_{13},r_{23},r_{12}), \qquad (10)$$

where N is the overall normalization factor. By means of the Galerkin method this equation is transformed into a generalized eigenvalue problem [22]:

$$\sum_{n_1,n_2,n_3} [\hat{H} - E\hat{S}] c^{n_1n_2n_3}_{ijk} = 0, \qquad (11)$$

where the coefficients $c^{n_1n_2n_3}_{ijk}$ are the eigenvectors and E the eigenvalues for the three-body system. Only one diagonalization is required and no further optimization process is needed. The overall amount of correlation included in the trial wave function is dictated by the number M of linear coefficients $c^{n_1n_2n_3}_{ijk}$. According to this number M a certain amount of excited states $n\,^{1,3}S$ states is also automatically obtained.

One final remark: Going beyond two-electron systems or S states is best tackled with a standard configuration interaction scheme involving only the electron-nucleus radial coordinates. The electron-electron interaction needs then special numerical attention. For unscreened Coulomb potential $U_{12}(r_{12})$ the well known multipole expansion is applicable. For screened cases, a special treatment is required; Ref. [25] addresses this issue showing how to accurately compute the corresponding matrix elements. For the present purposes, i.e., for three-body S states, our proposal of using explicitly the three interparticle coordinates avoids such numerical difficulties.

TABLE I. The mean energy and the mean of several radial quantities $\langle r^p_{ij}\rangle$ for the ground state of the negative ion H^- calculated with Ψ_{14}, for SCP and ECSCP models corresponding to several values of the screening parameter λ.

λ/Z	Model	$\langle -E\rangle$	$\langle r_{i3}\rangle$	$\langle r^2_{i3}\rangle$	$\left\langle \frac{1}{r_{i3}}\right\rangle$	$\langle r_{12}\rangle$	$\langle r^2_{12}\rangle$	$\left\langle \frac{1}{r_{12}}\right\rangle$
0.00		0.52644	2.55362	9.77238	0.69113	4.11824	21.0026	0.32312
		0.52775[a]	**2.71018**[a]	**11.9137**[a]	**0.68326**[a]	**4.41269**[a]	**25.2020**[a]	**0.31102**[a]
0.05	**SCP**	0.47724	2.81897	12.0299	0.67779	3.96205	19.1993	0.33011
		0.47903[c]						
	ECSCP	0.47643	2.82239	12.0087	0.67229	3.96356	19.218	0.33012
		0.47772[b]	**2.71067**[b]	**11.9220**[b]	**0.68328**[b]	**4.41293**[b]		**0.31103**[b]
0.1	**SCP**	0.43192	2.87736	12.3415	0.65147	3.99701	19.563	0.32771
		0.43295[c]						
	ECSCP	0.42650	2.90166	12.407	0.63454	4.00409	19.6468	0.32748
		0.42768[b]	**2.71723**[b]	**12.0145**[b]	**0.68304**[b]	**4.42143**[b]		**0.31074**[b]
0.25	**SCP**	0.30728	3.08474	13.7808	0.59032	4.15002	21.136	0.31630
		0.31074[c]						
	ECSCP	0.28049	3.15327	14.1312	0.55410	4.14588	21.1996	0.31795
		0.28160[b]	**2.87112**[b]	**13.9997**[b]	**0.67090**[b]	**4.67076**[b]		**0.29999**[b]
0.3	**SCP**	0.27655	3.15965	14.3574	0.57303	4.21685	21.8281	0.31134
	ECSCP	0.23422	3.22961	14.7887	0.53747	4.2162	21.9953	0.31354
0.4	**SCP**	0.20883	3.31867	15.6316	0.54003	4.37458	23.486	0.30002
	ECSCP	0.12919	3.30878	15.7536	0.52634	4.40195	24.1721	0.30295
0.5	**SCP**	0.15156	3.48678	17.0240	0.50819	4.56142	25.5040	0.28738
		0.15783[c]						
	ECSCP	0.04349	3.01915	14.2001	0.58633	4.75916	28.7088	0.28631
		0.08289[b]	**4.44800**[b]		**0.55593**[b]	**7.42501**[b]		**0.21233**[b]
0.6	**SCP**	0.10333	3.66032	18.4876	0.47706	4.7789	27.8938	0.27402
	ECSCP	0.01624	4.54579	25.7657	0.38649	5.42261	34.2274	0.22151

[a] G. W. F. Drake [26].
[b] A. Ghoshal and Y. K. Ho [14].
[c] S. Kar and Y. K. Ho [27].

III. RESULTS

We shall consider the first three two-electron systems ($z_1 = z_2 = -1$) with a nucleus of charge $z_3 = Z$: the negative ion H^- ($z_3 = 1$), the helium atom He ($z_3 = 2$), and the positive ion Li^+ ($z_3 = 3$), all considered with a virtual infinite mass nucleus ($m_3 \to \infty$); the reduced masses are simply $\mu_{13} = \mu_{23} = m_1 = m_2 = 1$, $\mu_{12} = 1/2$. We first study the ground state $1\,^1S$ (Sec. III A), and then the first excited state $n\,^1S$ and $n\,^3S$ for He and Li^+ (Sec. III B).

We shall consider the three potentials C, SCP, and ECSCP described in the Introduction, with three identical screening parameters $\lambda_{ij} = \lambda$, and $\delta_{ij} = \delta = \lambda$. This means, similarly to previous publications on the subject, that we assume screening effects apply equally to all pairs of charged particles. This allows us to compare our results with previously published reference values when available. The values for the pure Coulomb potential are well known (see, e.g., Ref. [26]) and can be considered as a special case of the SCP or ECSCP with zero screening parameters. For the ECSCP case—which is the main purpose of this work—comparison can be made with the results published by Ghoshal and Ho [8,14] obtained with highly correlated Hylleraas functions. At this point, it is worth recalling that the SCP and ECSCP are model potentials; hence, obtaining a great numerical precision may not be so crucial for some applications. Moreover, due to the large number of λ and/or δ values one may want to consider, a simpler (though sufficiently accurate) trial wave function may be sufficient.

One more remark: It is well known that for two-electron systems the coordinates may be rescaled with the nuclear charge Z, i.e., $r \to Zr$. Since screening intervenes in the potential through the product λr, it is natural to use λ/Z rather than λ as a variable parameter. Indeed, we found this variable to be appropriate, and should be useful in particular in applications where many isoelectronic species are to be studied.

A. Ground state $1\,^1S$

As only the ground states are considered in this section, the principal quantum numbers n_1 and n_2 are both set equal to 1 when building the wave functions (10). This leaves the choice of N_i, N_j, N_k, and n_3. To keep the trial wave functions reasonably simple and, at the same time, sufficiently accurate, we decided to perform all our calculations with n_3, N_1, N_2, and N_3 up to 2. We have thus considered the following wave function with 14 coefficients (parameters):

$$\begin{aligned}\Psi_{14} = N\,\{&\varphi_1(r_{13})\,\varphi_1(r_{23})\;{}_1F_1(-1,2,-2z_1z_2\mu_{12}r_{12})\\ &\times\left[c^{111}_{000} + c^{111}_{200}\left(r^2_{13}+r^2_{23}\right) + c^{111}_{220}r^2_{13}r^2_{23} + c^{111}_{300}\left(r^3_{13}+r^3_{23}\right)\right.\\ &\left. + c^{111}_{002}r^2_{12} + c^{111}_{202}\left(r^2_{13}+r^2_{23}\right)r^2_{12} + c^{111}_{222}r^2_{13}r^2_{23}r^2_{12}\right]\\ &+\varphi_1(r_{13})\,\varphi_1(r_{23})\;{}_1F_1(-2,2,-z_1z_2\mu_{12}r_{12})\\ &\times\left[c^{112}_{000} + c^{112}_{200}\left(r^2_{13}+r^2_{23}\right) + c^{112}_{220}r^2_{13}r^2_{23} + c^{112}_{300}\left(r^3_{13}+r^3_{23}\right)\right.\\ &\left. + c^{112}_{002}r^2_{12} + c^{112}_{202}\left(r^2_{13}+r^2_{23}\right)r^2_{12} + c^{112}_{222}r^2_{13}r^2_{23}r^2_{12}\right]\}. \quad (12)\end{aligned}$$

In Tables I, II, and III we present the calculated ground-state energies and the mean of radial quantities obtained with Ψ_{14}, for H^-, He, and Li^+. Results are given for several λ values in both SCP and ECSCP cases. Our $\lambda = 0$ results are compared with reference data [26]. Note that the Tables' entry is λ/Z and values larger than 0.6 are not included as the ECSCP energy is close to zero (see below). The ground-state energies of two-electron atoms lie below that of the corresponding one-electron atoms (e.g., He^+ for He or H for H^-). While this is well known for the pure Coulomb case, it was verified that this holds true also for SCP and ECSCP.

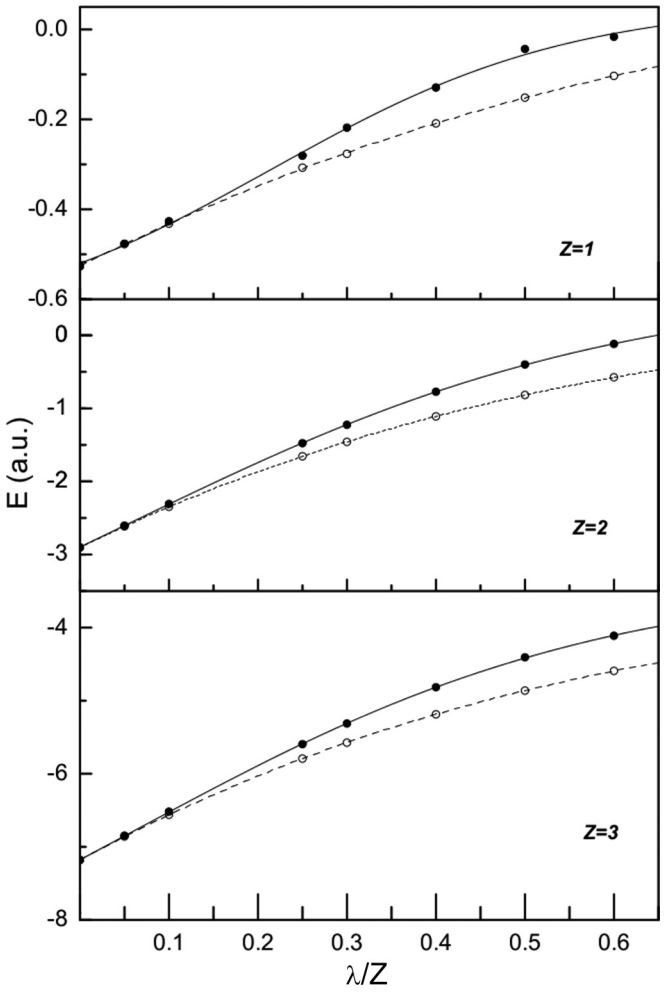

FIG. 1. Ground-state energy for H^-, He, and Li^+ in ECSCP and SCP for different values of the screening parameter λ. Calculations with the wave function (12) in ECSCP (solid circles) and SCP (open circles). The solid (respectively dashed) line correspond to a fit Eq. (13) of the calculated data for the ECSCP (respectively SCP) cases.

From the mathematical form of the two-body interactions, as a general trend, the overall potential strength decreases when going from pure Coulomb potentials to SCP and to ECSCP. Physically we therefore expect for screened potentials that the energy levels and the mean values $\langle r^p_{ij}\rangle(\lambda)$ for $p = 1,2$ to increase as λ increases (the reverse is true for $p = -1$ and -2). Besides, due to stronger screening effects, for a given λ the ECSCP values should lie above the corresponding SCP data. These trends are illustrated through the following figures. Figure 1 shows the calculated ground-state energy for $Z = 1,2,3$: it increases with the screening parameter, similarly for the two model potentials, but more strongly for ECSCP than for

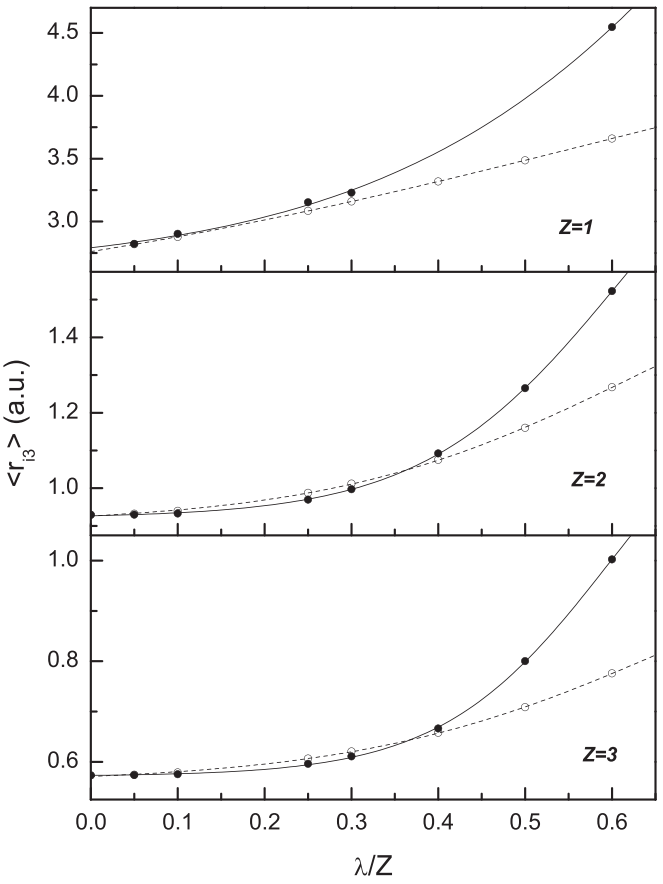

FIG. 2. Same as Fig. 1 but for the mean value of $\langle r_{i3}\rangle$.

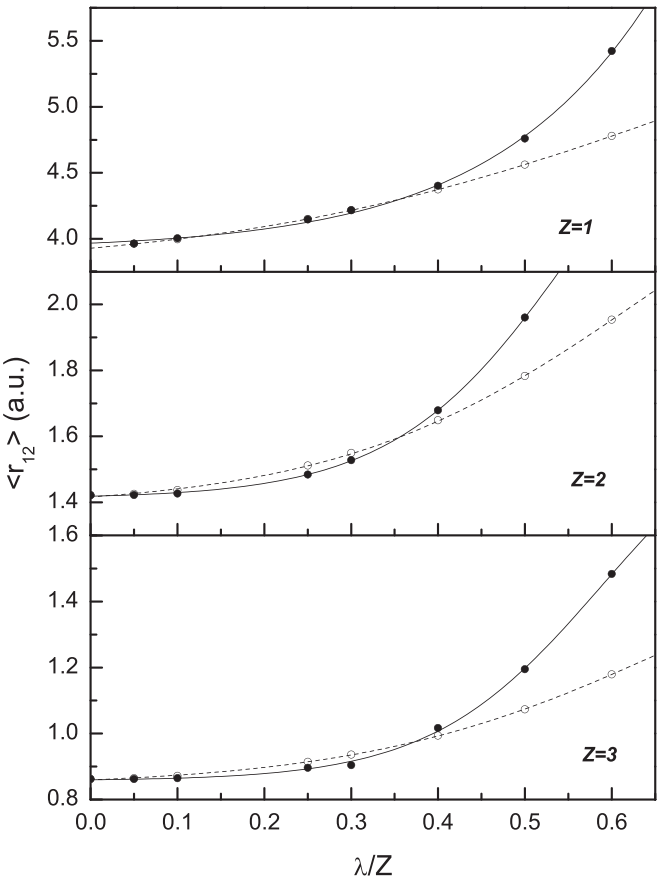

FIG. 3. Same as Fig. 1 but for the mean value of $\langle r_{12}\rangle$.

SCP. Clearly, for λ/Z just over 0.6 the ECSCP ground state ceases to exist (see also below). In Fig. 2 we show similar plots, but for the mean electron-nucleus distance $\langle r_{i3}\rangle$. Here we observe an important increase with λ/Z, meaning that as screening increases the electrons tend to be further away from the nucleus; this translates into overall larger two-electron systems. For $\lambda/Z > 0.35$, the effect is dramatically stronger for the ECSCP than for the SCP. The mean electron-electron distance $\langle r_{12}\rangle$ follows a similar trend (Fig. 3). This means that, compared to the pure Coulomb case, all three particles tend to separate further from each other when λ increases, and the system is only loosely bound. This trend accelerates as λ approaches the critical value λ_c for which the three-body system ceases to exist. One consequence of such changes into the atomic structure (not so deep ground state or, equivalently, larger size), is that the calculations with a limited number of basis functions may not be so accurate for increasing λ and in particular close to λ_c.

Let us now compare our results with those available in the literature. It is worth noting that, as it is always the case for two-electron atoms, simple trial wave functions provide better values with increasing nuclear charge as the electron-nucleus attraction dominates and the electron-electron correlation is then relatively less important. For H^-, our SCP energy results can be compared with those of Kar and Ho [27] (which are in practically perfect agreement with previous calculations of Winkler [28]); for ECSCP, our results (energy and other expectation values) can be compared with those of Ghoshal and Ho [14]. The agreement can only be considered as fair, and it gets worse as λ increases; one should keep in mind that we are comparing here our 14 parameter trial wave functions with highly correlated ones, for example with up to 525 terms [14]. For He, only the ECSCP energy values of Ghoshal and Ho [8] could be found in the literature. Agreement is very good, with relative energy differences of the order of 0.1%. (There is one exception, at $\lambda/Z = 0.5$, where our ECSCP energy value differs substantially more from Ghoshal and Ho result. We have verified our numbers, and suspect a zero is missing in Ref. [8].) For the SCP several calculations have been published and we have chosen to put in Table II those of Kar and Ho [9] obtained with 700 correlated basis functions (they coincide for example with those of Hashino *et al.* [29] within the six digits presented) and those of Lin *et al.* [10] obtained with about 4000 configurations (uncorrelated basis functions). In this case the relative difference is very small, ranging from 0.01% ($\lambda = 0$) to 0.15% ($\lambda = 0.6$). Note also that our results are only slightly above those of Lin *et al.* obtained with a very large number of uncorrelated basis functions. For mean values other than the energy, as the $\lambda = 0$ comparison is also very favorable, we believe our $\lambda \neq 0$ estimates should be reliable. Finally, except for the pure Coulomb case, no Li^+ could be found in the literature for comparison. The figures show no substantial difference with the screening trends observed for H^- or He.

One of the aims of this contribution is to provide an easy to use tool to estimate the energy $E(\lambda)$, or other expectation

TABLE II. Same as Table I but for the ground state He atom.

λ/Z	Model	$\langle -E \rangle$	$\langle r_{i3} \rangle$	$\langle r_{i3}^2 \rangle$	$\left\langle \frac{1}{r_{i3}} \right\rangle$	$\langle r_{12} \rangle$	$\langle r_{12}^2 \rangle$	$\left\langle \frac{1}{r_{12}} \right\rangle$
0.00		2.90337	0.92947	1.19281	1.68730	1.42163	2.51472	0.94632
		2.90372[a]	**0.92947**[a]	**1.19348**[a]	**1.68832**[a]	**1.42207**[a]	**2.51644**[a]	**0.94582**[a]
0.05	**SCP**	2.61451	0.93215	1.20082	1.68406	1.42576	2.53043	0.94397
		2.61485[b]						
		2.61471[c]						
	ECSCP	2.60409	0.92989	1.19418	1.68690	1.42228	2.51728	0.94601
		2.60444[d]						
0.1	**SCP**	2.34666	0.93961	1.22312	1.67498	1.43728	2.57441	0.93744
		2.34701[b]						
		2.34686[c]						
	ECSCP	2.30876	0.93257	1.20284	1.68417	1.42639	2.53354	0.94380
		2.30911[d]						
0.25	**SCP**	1.65504	0.98737	1.36956	1.61846	1.51143	2.86578	0.89736
		1.65540[b]						
	ECSCP	1.47653	0.96961	1.32342	1.64626	1.48410	2.76613	0.91417
		1.47696[d]						
0.3	**SCP**	1.45816	1.01184	1.44731	1.59093	1.54960	3.02149	0.87806
	ECSCP	1.22499	0.99730	1.41655	1.61893	1.52776	2.94860	0.89308
0.4	**SCP**	1.10973	1.07523	1.65701	1.52386	1.64886	3.44391	0.83149
	ECSCP	0.77276	1.09203	1.75299	1.53235	1.67894	3.61778	0.82701
0.5	**SCP**	0.81704	1.16018	1.95430	1.44189	1.78267	4.04953	0.77552
		0.81821[b]						
	ECSCP	0.40056	1.26525	2.41853	1.39272	1.95981	4.98046	0.72354
		0.40526[d]						
0.6	**SCP**	0.57486	1.26779	2.35204	1.34758	1.95356	4.87550	0.71262
	ECSCP	0.11843	1.52248	3.7167	1.20724	2.38538	7.27799	0.59614

[a]G. W. F. Drake [26].
[b]S. Kar and Y. K. Ho [9].
[c]Y. C. Lin *et al*. [10].
[d]A. Ghoshal and Y. K. Ho [8].

TABLE III. Same as Table I but for the ground state of the positive ion Li^+.

λ/Z	Model	$\langle -E \rangle$	$\langle r_{i3} \rangle$	$\langle r_{i3}^2 \rangle$	$\left\langle \frac{1}{r_{i3}} \right\rangle$	$\langle r_{12} \rangle$	$\langle r_{12}^2 \rangle$	$\left\langle \frac{1}{r_{12}} \right\rangle$
0.00		7.27948	0.57285	0.44637	2.68651	0.86224	0.92709	1.56829
		7.27991[a]	**0.57277**[a]	**0.44628**[a]	**2.68792**[a]	**0.86231**[a]	**0.92706**[a]	**1.56772**[a]
0.05	**SCP**	6.55753	0.57440	0.44914	2.68140	0.86463	0.93259	1.56456
	ECSCP	6.53007	0.57355	0.44761	2.68243	0.86189	0.92694	1.56968
0.1	**SCP**	5.88843	0.57873	0.45689	2.66709	0.87130	0.94802	1.55416
	ECSCP	5.79220	0.57512	0.45068	2.6783	0.86431	0.93272	1.56622
0.25	**SCP**	4.16097	0.60639	0.50776	2.57876	0.91405	1.04980	1.49070
	ECSCP	3.71497	0.59594	0.48854	2.61938	0.89603	1.00921	1.52039
0.3	**SCP**	3.66896	0.620589	0.53488	2.53587	0.93605	1.10424	1.46011
	ECSCP	3.07957	0.61077	0.51002	2.50806	0.90423	1.01821	1.48636
0.4	**SCP**	2.79753	0.65762	0.60889	2.43131	0.99362	1.25322	1.38601
	ECSCP	1.96141	0.67885	0.66631	2.42542	1.01653	1.33019	1.37679
0.5	**SCP**	2.06461	0.70842	0.71746	2.30234	1.07306	1.47337	1.29554
	ECSCP	1.04167	0.80017	0.94275	2.16706	1.19479	1.85681	1.19911
0.6	**SCP**	1.45791	0.77576	0.87188	2.15074	1.17927	1.79105	1.19066
	ECSCP	0.37758	1.00236	1.42967	1.77679	1.48329	2.80910	0.96744

[a]G. W. F. Drake [26].

TABLE IV. For the SCP potential, and for $Z = 1,2,3$, the fitting parameters a, A, B, C of Eq. (13) are given for the energy $\langle E\rangle$, and the mean values $\langle r_{i3}\rangle$ and $\langle r_{12}\rangle$.

$\langle f\rangle$	Z	a	A	B	C
$\langle E\rangle$	1	1.9199	0.4767	−2.6148	3.0661
	2	2.2780	1.5234	−14.020	3.3076
	3	2.2653	3.8441	−35.383	3.3364
$\langle r_{i3}\rangle$	1	2.3121	1.2721	2.1671	0.2457
	2	5.6532	0.0481	0.9047	0.0283
	3	5.4579	0.0275	0.5578	0.0248
$\langle r_{12}\rangle$	1	3.7646	0.4553	3.7604	0.0730
	2	5.6580	0.0725	1.3833	0.0273
	3	5.4469	0.0411	0.8389	0.0239

values, as a function of λ for both SCP and ECSCP models. To achieve this we propose analytical fits of mean values $\langle f\rangle$ in the form

$$\langle f\rangle_{\rm fit}(\lambda/Z) = \frac{A + B\, e^{-a(\lambda/Z)}}{C + e^{-a(\lambda/Z)}}. \tag{13}$$

The fitting parameters a, A, B, and C for the energy $\langle E\rangle$, and the mean values $\langle r_{i3}\rangle$ and $\langle r_{12}\rangle$, are given for the SCP (Table IV) and ECSCP (Table V) cases. Thus, for the first three Z values, one can estimate these mean values for any screening parameter λ by applying the fitting formula. The data obtained in this way are shown with solid (respectively, dashed) lines for ECSCP (respectively, SCP) in Figs. 1–3.

Next, we have searched the critical value λ_c of the screening parameter for which the ground state ceases to exist, and this for several nuclear charges Z ($Z < 20$ as relativistic effects may come into play for larger values). To do this we varied systematically, with successive fine tuning, the λ value of the ECSCP potential to find the one such that $\langle E\rangle(\lambda_c) = 0$. As this required quite a large number of calculations we have used a simpler trial wave function, namely the four parameters function (Ψ_4) given by (12) retaining only the coefficients c_{000} and c_{200}. The results are given in Table VI from which we observe that as Z increases so does λ_c; however, the ratio λ_c/Z is rather constant, especially for large nuclear charges. Through a linear fit of the data presented in the Table, we obtained the simple formula

$$\lambda_c = 0.66247Z - 0.07461, \tag{14}$$

TABLE V. Same as Table IV but for the ECSCP potential.

$\langle f\rangle$	Z	a	A	B	C
$\langle E\rangle$	1	5.9105	0.0169	−0.6849	0.2825
	2	3.5670	0.5862	−5.9201	0.8388
	3	3.7816	1.1359	−14.1304	0.7874
$\langle r_{i3}\rangle$	1	4.2183	0.2559	2.5977	0.0222
	2	8.8873	0.0097	0.9213	0.0045
	3	10.335	0.0030	0.5712	0.0021
$\langle r_{12}\rangle$	1	5.5246	0.0549	3.9099	0.00004
	2	9.6581	0.0131	1.4119	0.0044
	3	10.215	0.0050	0.8568	0.0025

TABLE VI. The value of the screening parameter λ_c for which $\langle E\rangle(\lambda_c) \simeq 0$, i.e., when the ground state ceases to exist for the ECSCP, is given for several nuclear charges Z. The last column provides the mean energy (not exactly zero as further λ fine tuning would be needed). Three additional entries (noted "Fit") are the values estimated by using Eq. (15).

Z		λ_c	λ_c/Z	$\langle E\rangle$
1		0.6000	0.6000	−0.00306
	Fit, Eq. (15)	0.6263	0.6263	0
2		1.250	0.625	−0.00929
	Fit, Eq. (15)	1.297	0.6483	0
3		1.915	0.6383	−0.00228
	Fit, Eq. (15)	2.000	0.6666	0
4		2.575	0.6437	−0.00524
5		3.237	0.6474	−0.00572
8		5.225	0.6531	−0.00727
10		6.549	0.6549	−0.00706
15		9.865	0.6577	−0.00370
17		11.185	0.6579	−0.05722
20		13.176	0.6588	−0.00609

which provides a reasonable estimate of the screening parameter value at which bound two-electron atoms of nuclear charge Z cease to exist. We have also evaluated the critical value by using the fit (13) for the energy; in this case λ_c is given by

$$\frac{\lambda_c}{Z} = -\frac{1}{a}\ln\left(\frac{-A}{B}\right). \tag{15}$$

The corresponding ECSCP values for $Z = 1,2,3$ are given in Table VI [similarly, for the SCP model, λ_c values can be easily calculated with Eq. (15)]. Note that precise numerical agreement with the previous λ_c values (obtained with Ψ_4) is not expected since the quality of the trial wave function is not the same.

B. Excited states $n\,^{1,3}S$

As we want to obtain approximate wave functions for the excited states $n\,^1S$ and $n\,^3S$ ($n = 2,3$), we have performed calculations with n_1 and n_2 up to 3, and included the following configurations:

$$1s1s + (1s2s + 2s1s) + (1s3s + 3s1s). \tag{16}$$

Satisfactory convergence was obtained with $n_3 = 1,2$ and $\Omega^{(N_i,N_j,N_k)}_{n_1,n_2,n_3}(r_{13},r_{23},r_{12}) = c^{n_1,n_2,n_3}_{000} + c^{n_1,n_2,n_3}_{200}(r^2_{13} + r^2_{23})$, i.e., with $M = 16$ coefficients; this choice keeps the approximated functions reasonably simple and, at the same time, sufficiently accurate. Our energy results are given in Table VII, for He and Li^+. Similarly to what is observed for the ground state, the energy levels increase with the screening parameter λ, and the effect is stronger for the ECSCP than for the SCP. As already commented for the ground state, when λ increases the three-body atomic system is larger in size, and less and less bound, so that a simple trial wave function may not be reliable enough in particular for excited states.

Comparison with published data [9,29] could be made only with SCP and only for the first excited states $2\,^1S$ and $2\,^3S$

TABLE VII. The mean energy of the excited $2^{1,3}S$ and $3^{1,3}S$ states of He and Li^+ calculated with a 16 terms wave trial wave function for the SCP and ECSCP models corresponding to several values of the screening parameter λ.

		He				Li^+			
λ/Z		$\langle -E\rangle_{2^3S}$	$\langle -E\rangle_{2^1S}$	$\langle -E\rangle_{3^3S}$	$\langle -E\rangle_{3^1S}$	$\langle -E\rangle_{2^3S}$	$\langle -E\rangle_{2^1S}$	$\langle -E\rangle_{3^3S}$	$\langle -E\rangle_{3^1S}$
0.00		2.17502	2.14571	2.06808	2.05978	5.11033	5.04028	4.75192	4.73340
		2.17523[a]	**2.14597**[a]	**2.06869**[a]	**2.06127**[a]	**5.11072**[a]	**5.04088**[a]	**4.75208**[a]	**4.73375**[a]
0.05	**SCP**	1.90082	1.87481	1.81338	1.80667	4.42550	4.36097	4.12082	4.10721
		1.9010[b]	**1.8750**[b]						
		1.90101[c]	**1.87504**[c]						
		1.90101[d]	**1.87503**[d]						
	ECSCP	1.88096	1.85374	1.79158	1.78527	4.37399	4.30690	4.05936	4.04662
0.1	**SCP**	1.66992	1.65127	1.61293	1.60647	3.85126	3.79972	3.64700	3.63798
		1.6703[b]	**1.6509**[b]						
		1.67010[c]	**1.65149**[c]						
		1.67010[d]	**1.65149**[d]						
	ECSCP	1.61543	1.59988	1.57549	1.56783	3.70341	3.65307	3.55163	3.54446
0.25	**SCP**	1.15629	1.15339	1.12322	1.11547	2.61001	2.60187	2.53931	2.52489
		1.16384[c]	**1.16375**[c]						
	ECSCP	1.03402	1.03327	0.99228	0.98811	2.32594	2.32480	2.23112	2.22442
0.3	**SCP**	1.02005	1.01833	0.98477	0.97783	2.29970	2.29489	2.22369	2.21092
		1.0168[b]	**1.0116**[b]						
	ECSCP	0.86456	0.86375	0.82222	0.81837	1.94481	1.94362	1.84818	1.84256
0.4	**SCP**	0.78003	0.77803	0.73806	0.73122	1.75689	1.75341	1.66782	1.65701
		0.7770[b]	**0.7720**[b]						
	ECSCP	0.55513	0.55373	0.51149	0.50631	1.24880	1.24675	1.14960	1.14228
0.5	**SCP**	0.57636	0.57388	0.52940	0.52159	1.29780	1.29373	1.19593	1.18410
		0.5747[b]	**0.5694**[b]						
		0.59258[c]	**0.59255**[c]						
	ECSCP	0.29092	0.28772	0.24229	0.23252	0.65437	0.64957	0.54397	0.52911
0.6	**SCP**	0.40535	0.40191	0.35340	0.34352	0.91224	0.906634	0.79516	0.77947
	ECSCP	0.07811	0.06995	0.01917	–	0.17560	0.16192	0.04163	0.00432

[a]G. W. F. Drake [26].
[b]T. Hashino *et al*. [29].
[c]S. Kar and Y. K. Ho [9].
[d]Y. C. Lin *et al*. [10].

of He. While for $\lambda = 0$ agreement is more than satisfactory, the same cannot be stated as λ increases indicating that our modest 16 term trial wave functions may not be sufficiently accurate when compared to calculations using several hundred explicitly correlated basis functions (444 for [29] and 700 for [9]) or several thousand uncorrelated ones [10]. This said, we should note here that it is not easy to assert which SCP values should be considered as benchmarks. For $\lambda/Z = 0.5$, for example, our energy values are better and closer than those of the older reference [29] but worse than those of Ref. [9] (the latter energies are lower and should thus be considered as better ones). For $\lambda/Z = 0.4$ and 0.3, our energy values are better than those of Ref. [29]. For $\lambda/Z = 0.1$ our results are quite close ($\sim$0.01% difference) to those of the more recent references [9,10], but for the $2\,^3S$ state, Hashino *et al*. [29] published a lower value. (Since three different calculations seem consistent with each other, one may suspect a typographical mistake associated to the -1.6703 energy value [29]).

Finally, in Ref. [9] it was noted that for He in SCP the energy split $E(2\,^3S)$-$E(2\,^1S)$ between the first two excited states decreases with λ. Except for $\lambda/Z > 0.3$, a similar trend is observed here also in the case of ECSCP, both for He and Li^+ (Here we should note that, in view of the above SCP comparison with the sophisticated calculations of Ref. [9], our excited states energy $\lambda/Z > 0.3$ may not be accurate enough). The data analysis of Table VII shows, on the other hand, that the split $E(3\,^3S)$-$E(3\,^1S)$ does not present at all such a trend in either SCP or ECSCP.

IV. SUMMARY

We have studied two-electron atoms embedded in a plasma environment. According to the plasma density, the three two-body interactions can be modeled through screened Coulomb potentials. As these are models, and great precision may not be needed, we have employed rather simple—though accurate enough—trial wave functions. These allowed us to perform a systematic study, for example, of the critical screening value at which the ground state ceases to exist, or to get practical fits of mean values, and this for several nuclear charges. Our investigation led us to identify the ratio λ/Z, rather than λ, as a natural parameter. The proposed three-body wave

function is built within a configuration interaction scheme with parameter-free explicitly correlated basis functions. Since all included parameters are linear, a single diagonalization provides both energies and eigenvectors of the ground and a number of excited S states of the system. The energies of the excited states $2\,^{1,3}S$ and $3\,^{1,3}S$ for He and Li^+ in the ECSCP model are given here.

As previous publications on three-body ECSCP, we have used the same screening parameter $\lambda = \delta$ for all three interactions between pairs of charged particles. For a given physical problem, whether in plasma, solid-state, or nuclear physics, the ECSCP model potential may require assuming the more general case in which the three pairs are not treated equally and/or $\lambda \neq \delta$ (for the two-body interaction, Roy [30] suggests the general case $\lambda \neq \delta$, but then provides very precise calculations only for $\lambda = \delta$). Within the SCP picture, Certík and Winkler [25] considered the case of different Debye screening values for the electron-nucleus and electron-electron interactions; as the latter have opposing effects in lowering/increasing the energy, the interplay is of definite interest. With no extra effort, our versatile methodology applies equally well to these more general situations. Moreover, the relative simplicity of our proposed trial wave functions is ideally suited for calculations involving large numbers of screening parameters.

ACKNOWLEDGMENTS

We would like to thank G. Gasaneo for his remarks on the manuscript. This work has been developed within the activities planned in the French-Argentinian program ECOS-Sud A10E01. The support by ANPCyT (PICT08/0934) (Argentina) and PIP 200901/552 CONICET (Argentina) is acknowledged. K.V.R. also thanks the support by PGI 24/F049 Universidad Nacional del Sur (Argentina).

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