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Fine-structure quenching and multiplet distortion in a screened Coulomb atom

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Abstract. Theoretical results presented in this paper reflect that the relativistic fine-structure due to the mass-velocity, spin-orbit and Darwin terms is sensitive to the screening strength parameter in an exponential screened Coulomb hydrogen atom, that is sometimes used to model a plasma-embedded atom. With stronger screening the fine-structure correction undergoes a gradual suppression in magnitude, but contributes to the total binding energy in an increasing proportion, indicating that the relativistic contribution to binding may become quite significant in the ultra-low binding regime under large screening strength. In the presence of screening the l-independence of the fine-structure correction as predicted by the Dirac theory progressively disappears, and a departure from the Z^4-scaling law of the correction occurs along the H-isoelectronic sequence of ions – both the effects become accentuated with growing screening strength. In conjunction with screening-induced removal of the Coulomb degeneracy of non-relativistic levels, these result in a deformed multiplet structure for the screened Coulomb atom.

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1 Introduction

The exponential screened Coulomb atom represents a well-known paradigm where the idea of static (Debye) screening of a test charge within a plasma is directly transported to the constituent charges within an individual atom to approximately delineate the situation when the atom is embedded in a plasma. At least for classical charged particles, the effect of the plasma sea on localized two-particle interactions is to replace the Coulomb potential by an effective screened Coulomb one that is known in plasma physics as the Debye-Hückel potential [1] and is given by,

$$V^{\mathrm{D}}(r) = \pm e^2 \exp(-\mu r)/r \qquad (1)$$

where μ is the screening strength parameter, and the "−" ("+") sign denotes attractive (repulsive) interaction. In the past, the bound-state energies of an electron in the screened field of a proton (*i.e.*, the so-called "Debye-screened H-atom") had been calculated by a number of authors employing a variety of techniques [2–11]. These studies revealed that, (i) the screened H-atom has a finite eigenspectrum – the energy eigenvalues are function of the density and temperature, and (ii) the magnitude of the ionization energy reduces as the screening increases, which is more frequently referred to as the "continuum lowering" in the literature. Incorporating the screening for the electron-electron repulsion term too, the screened atom model had been extended earlier for calculation of ionization potential of the helium atom in a plasma [12]. Recent years have witnessed a number of studies within the framework of this Debye-screened model for the plasma-embedded atom, that consider the detachment energy and stability criterion of a negative hydrogen ion in plasmas [13], the excited states and the radiative transition properties of a plasma-perturbed stripped two-electron ion [14,15], as well as the screening-dependence of optical field ionization of ions induced by ultrashort laser pulses [16]. Besides, it may not be altogether out of place to mention here in passing that, the modification in bound electronic structure of a screened Coulomb atom has important consequences not only for the calculation of spectroscopic features, but also for the calculation of thermodynamic properties; in particular, the atomic partition function that determines the distribution of ionization through Saha's equation [17,18]. The use of the screened Coulomb potential model restricts the sum in the partition function to a finite number of terms that can be supported by the plasma, and thus removes the difficulty associated with the well-known divergence problem [5] of the same for a free Coulomb atom. We may note in this context that the formulation of the partition function in a dense plasma has been a subject of considerable debate in the literature [19].

However, it appears that only the non-relativistic atomic structures of the representative one- and two-electron screened Coulomb atoms have been explored in some detail up to now, and more subtle aspects like the

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relativistic fine-structure (which are integral part of an atomic spectra) in such screened atomic systems have not been touched upon so far. We recognize the fact that the presence of screening is liable to modify the fine-structure correction with possible interesting consequences in the associated multiplet structures, because this correction itself depends on the nature of the binding potential within the atom. In this connection first we recall that, for one-electron systems the fine-structure correction owes its origin to three [20] effects. These are,

(i) the mass-velocity correction, which arises due to relativistic variation of the electron mass with velocity, and is, in fact, a correction to the kinetic energy term in the non-relativistic Hamiltonian. It is expressed as,

$$H^{\mathrm{MV}} = -(1/2mc^2)[E - V(r)]^2; \tag{2a}$$

(ii) the spin-orbit correction, which represents the magnetic interaction energy between the electron's spin magnetic moment and the magnetic field that the electron experiences due to its orbital motion through the electric field of the nucleus, and is given by,

$$H^{\mathrm{SO}} = (\hbar^2/4m^2c^2)(2/r)[\mathrm{d}V(r)/\mathrm{d}r](\mathbf{l}\cdot\mathbf{s}); \tag{2b}$$

(iii) the Darwin correction [21], which has no classical analog and may be visualized as arising from a relativistically induced electric moment of the electron, or, be better interpreted in terms of the relativistic non-localizability of the electron [22,23]:

$$H^{\mathrm{D}} = -(\hbar^2/4m^2c^2)[\mathrm{d}V(r)/\mathrm{d}r](\partial/\partial r). \tag{2c}$$

All these three corrections are of the same order of magnitude, and therefore, must be treated together. However, they differ in signs, but their sum – the fine-structure correction, is always negative.

In equations (2a–2c) we note the presence of the central potential $V(r)$, its power and the first-derivative that make the operators explicitly screening-dependent for a screened Coulomb atom. Additionally, the (unperturbed) eigenfunctions of the screened Coulomb system that are required in case of a perturbative treatment of these correction terms are themselves implicit functions of the screening parameter. So, we find it worth-investigating in this article how these three comparable (and sometimes opposing due to the sign) corrections separately behave under screening, how their collective contribution comes in the screening-dependence of the fine-structure correction, and finally, its possible implications to the relativistic multiplet structures of the screened atom as well as to the variation of the fine-structure along the H-isoelectronic series of ions. Furthermore, the following point needs to be mentioned here: the relativistic fine-structure corrections in one-electron ions is known to be very small in magnitude compared to the non-relativistic energy in low-Z species, yet it increases the binding since it is negative and constitutes only a negligible fraction of the total binding energy for a Coulomb atom – the energies of the fine-structure multiplet members are all little lower than the non-relativistic energy of the atomic level in question. But, from the earlier calculations [2–11] of the non-relativistic energy of the screened H-atom it is known that, as the screening increases this energy grows until it becomes zero as the state finally becomes part of the continuum at a critical screening strength. In this near-threshold region with greatly reduced non-relativistic binding (that itself may here become comparable in magnitude to the fine-structure correction), it seems necessary to study the screening-dependent behavior of the fine-structure, because here such corrections may eventually turn out to be an important mechanism contributing substantially to the ultra-low total binding of a quasi-free level which is attached almost dissociatively to the atom. We have partially addressed this issue in our study. The screening effects on the hydrogenic fine-structures composed of the three components are explored in this calculation first by means of a perturbative scheme for the correction terms, and then the perturbatively-obtained fine-structure corrections are checked and compared against the "exact" ones obtained from the difference between the relativistic screened Coulomb Dirac eigenvalues and the corresponding non-relativistic screened Coulomb Schrödinger eigenvalues. In the next section the theoretical procedure followed here is outlined in brief, and this is followed by a presentation and discussion of the numerical results in the concluding section.

2 Theoretical model

For a perturbative treatment of the fine-structure comprised of the three correction terms in a Debye-screened hydrogen-like atomic ion with nuclear charge Z, the total perturbed Hamiltonian is partitioned in the usual way:

$$H = H^0 + H^{\mathrm{MV}} + H^{\mathrm{SO}} + H^{\mathrm{D}}, \tag{3}$$

where H^0 stands for the unperturbed Hamiltonian corresponding to the screened non-relativistic ion in which the Coulomb potential $V^{\mathrm{C}}(r) = -2Z/r$ (in Rydberg units) is replaced by a static screened Coulomb or, the "Debye" potential $V^{\mathrm{D}}(r;\mu) = -(2Z/r)\exp(-\mu r)$. The parameter μ is zero for no-screening in a free or isolated Coulomb system and increases continuously as the screening becomes stronger. Thus, by varying μ in steps a systematic study of the screening effects can be performed.

H^0 satisfies the non-relativistic time-independent Schrödinger equation valid for the Debye-screened atomic ion, leading to the radial equation given below following the standard separation of variable technique for the central field problems,

$$[-\mathrm{d}^2/\mathrm{d}r^2 + l(l+1)/r^2 - (2Z/r)\exp(-\mu r)]P_{nl}(r;\mu) = E_{nl}^{\mathrm{NR}}(\mu)P_{nl}(r;\mu). \tag{4}$$

Although a laborious analytic solution of equation (4) might be possible [8], such solutions may not be easily amenable to calculations of the matrix elements of different operators of physical interests in closed forms.

That's why, in this calculation numerical solutions to equation (4) are sought at specific values of the screening strength μ, so that the unperturbed eigenfunctions P_{nl} and the non-relativistic unperturbed eigenvalues E_{nl}^{NR} become implicitly dependent on μ. Also it is to be noted that the "accidental" or l-degeneracy in the eigenvalues of a Coulomb system is lifted in the present case, and the screened Coulomb eigenenergies in equation (4) depend on n and l both.

Now, within the framework of the first-order perturbation theory, the three corrections to the unperturbed energy E_{nl}^{NR} corresponding to the three operators mentioned in Section 1 are given by the expectation values of the relevant operators in the zeroth-order eigenstate (two-component spin-orbital), which entails the evaluation of the following radial integrals in the coordinate representation:

$$\Delta E_{nl}^{\mathrm{MV}}(\mu) = -(\alpha^2/4)\int_0^\infty P_{nl}^*(r;\mu) \times [E_{nl}^{\mathrm{NR}}(\mu) - V^{\mathrm{D}}(r;\mu)]^2 P_{nl}(r;\mu)\mathrm{d}r, \quad (5a)$$

$$\Delta E_{nlj}^{\mathrm{SO}}(\mu) = (\alpha^2/4)[j(j+1) - l(l+1) - s(s+1)] \times \int_0^\infty P_{nl}^*(r;\mu)(r^{-1}\mathrm{d}V^{\mathrm{D}}/\mathrm{d}r)P_{nl}(r;\mu)\mathrm{d}r, \quad (5b)$$

$$\Delta E_{nl}^{\mathrm{D}}(\mu) = -(\alpha^2/4)\int_0^\infty P_{nl}^*(r;\mu) \times (\mathrm{d}V^{\mathrm{D}}/\mathrm{d}r)r[\mathrm{d}(r^{-1}P_{nl})/\mathrm{d}r]\mathrm{d}r. \quad (5c)$$

So, the total energy corresponding to the total perturbed Hamiltonian H of the screened Coulomb ion, including the perturbatively-obtained fine-structure corrections $\Delta E_{nlj}^{\mathrm{PERT}}(\mu)$ (which is the sum of the three correction terms given in Eqs. (5a–5c)), may now be written (up to the first-order) as a function of the screening strength as,

$$\begin{aligned} E_{nlj}(\mu) &= E_{nl}^{\mathrm{NR}}(\mu) + \Delta E_{nlj}^{\mathrm{PERT}}(\mu) \\ &= E_{nl}^{\mathrm{NR}}(\mu) + \Delta E_{nl}^{\mathrm{MV}}(\mu) + \Delta E_{nlj}^{\mathrm{SO}}(\mu) + \Delta E_{nl}^{\mathrm{D}}(\mu). \end{aligned} \quad (6)$$

The symbols n, $\mathbf{l}$, l, $\mathbf{s}$, s, $\mathbf{j}$ $(= \mathbf{l} + \mathbf{s})$, j used so far are to be understood in their usual senses; besides, in equations (4–6) all the distances (r, μ^{-1}) are measured in atomic length units *i.e.* in units of the Bohr radius $a_0 = (\hbar^2/me^2) = 0.529\,177$ Å, all energies (including the Hamiltonians themselves) are expressed in Rydberg units of $(\hbar^2/2ma_0^2) = (e^2/2a_0) = 13.6058$ eV, angular momenta in units of $\hbar$, and the dimensionless fine-structure constant that controls the order of magnitudes of the fine-structure corrections is given by $\alpha = (e^2/c\hbar) = (\hbar/mca_0) = 1/137.036$, c being the velocity of light.

Finally, the accuracy of $\Delta E_{nlj}^{\mathrm{PERT}}(\mu)$ is judged against the "exact" fine-structure correction $\Delta E_{nlj}^{\mathrm{EXACT}}(\mu)$ which is given by the shift of the relativistic screened-Coulomb Dirac energy $E_{nlj}^{\mathrm{DIRAC}}(\mu)$ from the non-relativistic screened Coulomb Schrödinger energy for specific values of μ, *i.e.*, $\Delta E_{nlj}^{\mathrm{EXACT}}(\mu) = E_{nlj}^{\mathrm{DIRAC}}(\mu) - E_{nl}^{\mathrm{NR}}(\mu)$. For this purpose the radial Dirac equations ([24], Sect. 53) with a screened Coulomb potential are solved following the procedure of Salvat and Mayol [25] (for a pure Coulomb atom, *i.e.* for $\mu = 0$, the quantities ΔE^{PERT}, $\Delta E^{\mathrm{EXACT}}$, E^{NR}, E^{DIRAC} and E are all independent of l).

3 Results

We confine most of our discussion to the fine-structure levels pertaining to the principal quantum numbers $n = 1$, 2 and 3 in hydrogen as a typical representative case; the fine-structures in hydrogenic ions are only referred to in connection with the Z-dependence of the fine-structure correction (Fig. 4). Some of the quantitative results for the H-atom are quoted in Table 1, which are further highlighted graphically in the Figures 1–3. For the sake of convenience we have tabulated all the energy values in spectroscopic units of cm^{-1} (1 Rydberg = 109 737 cm^{-1}), while the screening strength parameter μ is retained in atomic units of length^{-1}. The gross effect of screening on a discrete atomic bound state is a gradual loss of its binding or, lowering of the ionization continuum with increasing screening until the state finally sinks in the continuum at a critical value of the screening strength. This gives rise to a finite number of bound states for the screened Coulomb atom and is indicated in Table 1 in the progressively reduced magnitudes of the non-relativistic energy E^{NR} of all the states concerned as μ becomes larger. The other important effect on E^{NR} is the lifting of l-degeneracy of the Coulomb levels by the introduction of screening, that manifests itself in Table 1 in the growing separation between the non-relativistic energies of different l-sublevels belonging to a specific n as μ increases. For the ground state of hydrogen the influence of screening on energy becomes highly conspicuous at $\mu \sim 0.5-1.0$ a.u. The higher excited states being more loosely bound are susceptible to the screening effects at relatively lower values of μ.

Since each of the three corrections in equations (5) depends both explicitly (through the corresponding operators) as well as implicitly (through the non-relativistic energies and radial functions) on the screening strength μ, it would be of interest to study initially their individual patterns of variation with μ in order to gather some idea about the separate contributions of these three components in the screening-dependence of the fine-structure correction ΔE^{PERT}. First, let us consider the "mass-velocity" term. From equation (5a) it is straightforward to show that for a Coulomb atom,

$$\Delta E_{nl}^{\mathrm{MV}}(\mu = 0) = -(\alpha^2 Z^4/4n^4)[4n/(l + 1/2) - 3]Ry, \quad (7a)$$

so, it depends on n and l both, and is always negative. This correction at $\mu = 0$, and at two other non-zero values of μ for the screened Coulomb atom is shown in Table 1 for all the levels concerned. In Figures 1a and 1b,

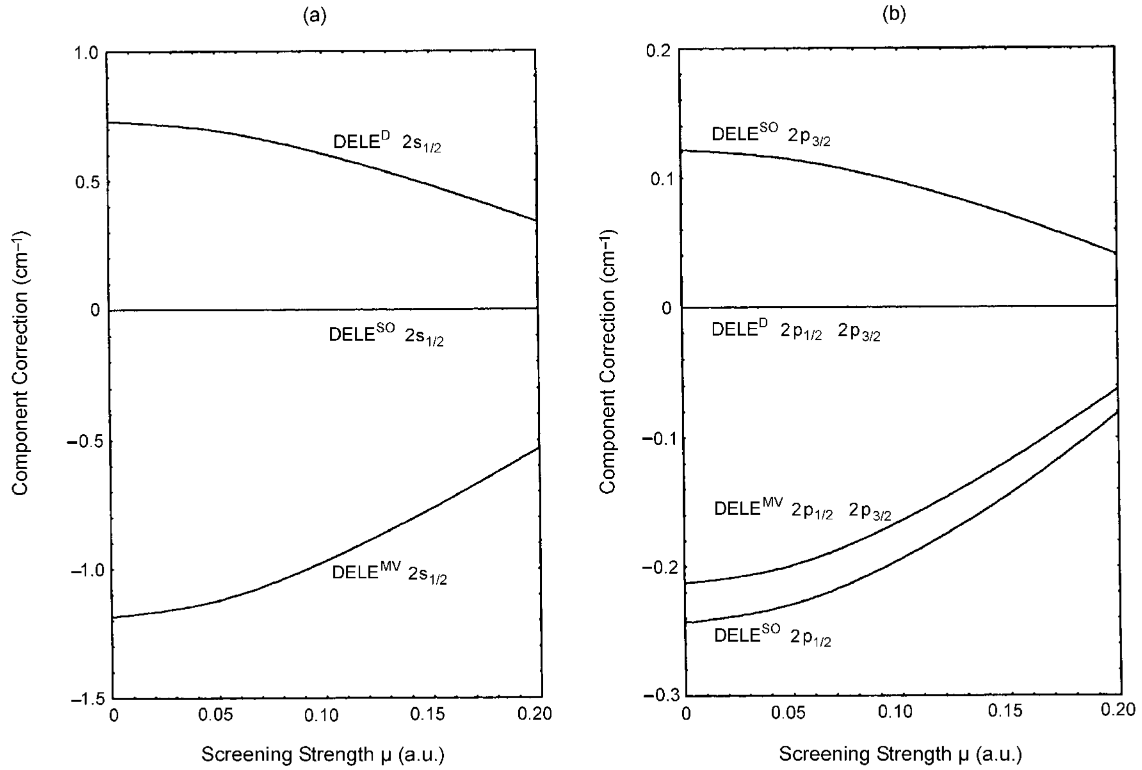

Fig. 1. Variation of the mass-velocity correction (ΔE^{MV}), the spin-orbit correction (ΔE^{SO}) and the Darwin correction (ΔE^{D}) with the screening strength μ for (a) the $2s_{1/2}$ level, and (b) the $2p_{1/2}$ and $2p_{3/2}$ levels of hydrogen.

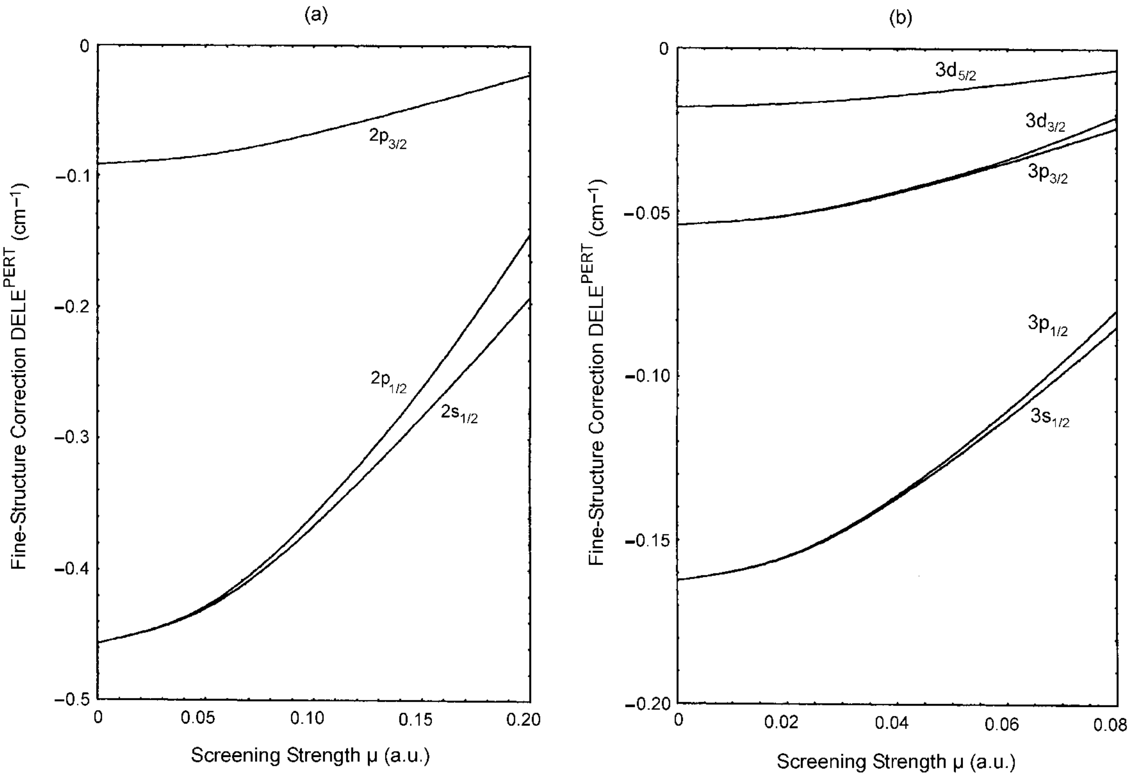

Fig. 2. Screening strength (μ)-dependence of the fine-structure correction (ΔE^{PERT}) for (a) the $n = 2$ fine-structure levels, and (b) the $n = 3$ fine-structure levels of hydrogen.

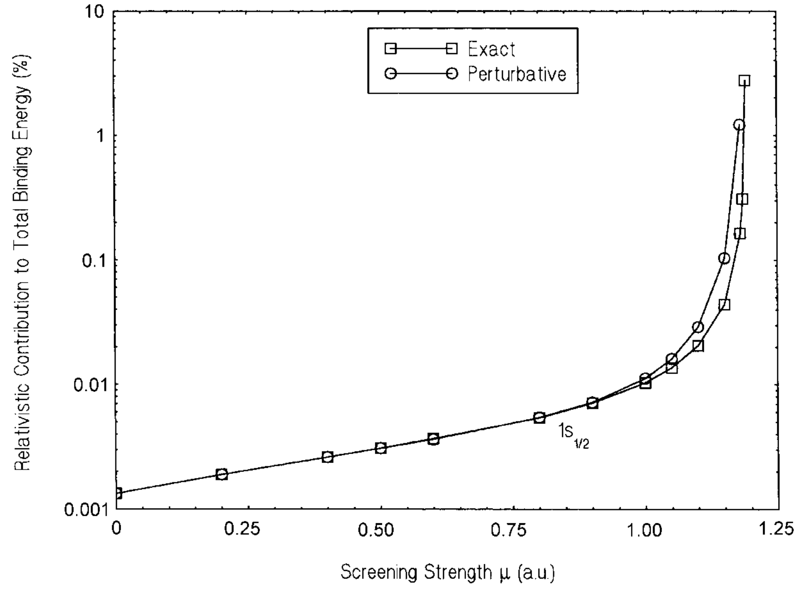

Fig. 3. Percent contribution of the relativistic fine-structure correction in the total binding energy for the $1s_{1/2}$ level of hydrogen as a function of the screening strength μ.

Table 1. The non-relativistic energy E^{NR} (cm^{-1}), the relativistic mass-velocity correction ΔE^{MV} (cm^{-1}), spin-orbit correction ΔE^{SO} (cm^{-1}), Darwin correction ΔE^{D} (cm^{-1}), the perturbatively-obtained fine-structure correction ΔE^{PERT} ($= \Delta E^{\mathrm{MV}} + \Delta E^{\mathrm{SO}} + \Delta E^{\mathrm{D}}$) (cm^{-1}) as well as the "exact" fine-structure correction $\Delta E^{\mathrm{EXACT}}$ (cm^{-1}) as a function of the screnning strength parameter μ (in atomic units of length^{-1}) for the ground and the first two excited states of hydrogen.

Level	$1s_{1/2}$	$2s_{1/2}$	$2p_{1/2}$	$2p_{3/2}$	$3s_{1/2}$	$3p_{1/2}$	$3p_{3/2}$	$3d_{3/2}$	$3d_{5/2}$
[n l j]	[1 0 1/2]	[2 0 1/2]	[2 1 1/2]	[2 1 3/2]	[3 0 1/2]	[3 1 1/2]	[3 1 3/2]	[3 2 3/2]	[3 2 5/2]
	μ= 0	μ= 0			μ= 0				
E^{NR}	-109737	-27434	-27434	-27434	-12193	-12193	-12193	-12193	-12193
ΔE^{MV}	-7.3046	-1.1870	-0.2130	-0.2130	-0.3787	-0.0902	-0.0902	-0.0325	-0.0325
ΔE^{SO}	0	0	-0.2435	0.1217	0	-0.0721	0.0361	-0.0216	0.0144
ΔE^{D}	5.8436	0.7305	0	0	0.2164	0	0	0	0
ΔE^{PERT}	-1.4610	-0.4565	-0.4565	-0.0913	-0.1623	-0.1623	-0.0541	-0.0541	-0.0181
$\Delta E^{\mathrm{EXACT}}$	-1.4610	-0.4565	-0.4565	-0.0913	-0.1623	-0.1623	-0.0541	-0.0541	-0.0181
	μ= 0.5	μ= 0.1			μ= 0.04				
E^{NR}	-32508	-10958	-10213	-10213	-5419.3	-5295.9	-5295.9	-5045.7	-5045.7
ΔE^{MV}	-5.1938	-0.9709	-0.1646	-0.1646	-0.3227	-0.0750	-0.0750	-0.0261	-0.0261
ΔE^{SO}	0	0	-0.1940	0.0970	0	-0.0613	0.0306	-0.0177	0.0118
ΔE^{D}	4.1965	0.6041	0	0	0.1856	0	0	0	0
ΔE^{PERT}	-0.9973	-0.3668	-0.3586	-0.0676	-0.1371	-0.1363	-0.0444	-0.0438	-0.0143
$\Delta E^{\mathrm{EXACT}}$	-0.9973	-0.3667	-0.3608	-0.0699	-0.1371	-0.1364	-0.0445	-0.0440	-0.0144
	μ= 1.0	μ= 0.2			μ= 0.08				
E^{NR}	-2257.3	-2657.2	-905.3	-905.3	-1706.4	-1389.3	-1389.3	-713.3	-713.3
ΔE^{MV}	-1.5131	-0.5324	-0.0628	-0.0628	-0.2037	-0.0427	-0.0427	-0.0121	-0.0121
ΔE^{SO}	0	0	-0.0814	0.0407	0	-0.0369	0.0184	-0.0087	0.0058
ΔE^{D}	1.2614	0.3405	0	0	0.1191	0	0	0	0
ΔE^{PERT}	-0.2517	-0.1919	-0.1442	-0.0221	-0.0846	-0.0796	-0.0243	-0.0208	-0.0063
$\Delta E^{\mathrm{EXACT}}$	-0.2329	-0.1910	-0.1458	-0.0253	-0.0844	-0.0798	-0.0245	-0.0210	-0.0065

it is plotted as a function of μ for the $n = 2$ multiplet members ($2s_{1/2}$, $2p_{1/2}$ and $2p_{3/2}$) in hydrogen. As can be seen from these figures, this correction smoothly rises up with the screening strength for all fine-structure levels; in addition, the trend of variation does not distinguish between the two different $j = l \pm 1/2$ levels.

Next we consider the "spin-orbit" correction. For an isolated Coulomb atom equation (5b) yields,

$$\begin{aligned}\Delta E^{\mathrm{SO}}_{nlj}(\mu = 0) = (1 - \delta_{l0})[\alpha^2 Z^4/n^3 l(l + 1)(2l + 1)]\\ \times\, lRy \quad \text{for} \quad j = l + 1/2\\ \times -[(l + 1)]Ry \quad \text{for} \quad j = l - 1/2 \end{aligned} \tag{7b}$$

where $\delta_{l0} = 1$ for $l = 0$ and $\delta_{l0} = 0$ for $l \neq 0$.

So, this correction depends on n, l as well as on j; for $l = 0$ it is zero, for $l \neq 0$ it is positive for higher j and negative for lower j and is displayed in Table 1 for the Coulomb as well as for the Debye-screened atom. From Figures 1a and 1b, this correction exhibits continuous variation with the screening strength – that corresponding to the higher j-value reduces with increasing μ, while the one for the lower-j increases as μ grows up.

From equation (5c) the third of these corrections *e.g.* the "Darwin correction" for a free Coulomb atom is given by,

$$\Delta E^{\mathrm{D}}_{nl}(\mu = 0) = \delta_{l0}(\alpha^2 Z^4/n^3)Ry. \tag{7c}$$

It is apparent that this correction depends on n and l, for $l = 0$ it is positive and for $l \neq 0$ it vanishes. This correction for the levels concerned is also tabulated for the Coulomb and the screened Coulomb cases in Table 1 and its screening-dependence is presented graphically in Figures 1a and 1b for the $n = 2$ fine-structure levels of hydrogen. Clearly, this correction decreases monotonically with growing screening strength.

From equations (7a–7c) one obtains the perturbative fine-structure correction for a Coulomb atom as the sum of the three correction terms,

$$\Delta E^{\mathrm{PERT}}_{nj}(\mu = 0) = -(\alpha^2 Z^4/4n^4)[4n/(j + 1/2) - 3]Ry. \tag{7d}$$

So, the total correction is always negative as the maximum value of $j + 1/2 = l + 1$ is n. Besides, all the three corrections are seen to depend on l, but in the sum the l-dependence is cancelled out so that the total correction becomes independent of l. As a consequence, a non-relativistic energy level E^{NR}_n corresponding to the principal quantum number n splits into n number of fine-structure levels (forming a multiplet), one for each value of the total angular momentum quantum number $j = 1/2$, $3/2$, ... $(n - 1/2)$; two states having the same value of the quantum numbers n and j but with two different values of $l = j \pm 1/2$ will have the same energy. The origin of such degeneracy of the fine-structure levels in the relativistic (Dirac) theory with a pure Coulomb potential can be traced to the commutation of the Hamiltonian with a scalar operator ([24], Sect. 53) in as much the same way as the "accidental" l-degeneracy for a pure Coulomb potential in the non-relativistic case may be connected to the commutation of the Hamiltonian with the Runge-Lenz vector ([24], Sect. 30); in both cases a different potential (a screened Coulomb one, for example) should remove the degeneracy (the degeneracy in the relativistic Coulomb case is however actually removed by quantum electrodynamic effect *e.g.* the Lamb shift, which we do not delve into at present). It is demonstrated in Table 1 for $\mu = 0$, where the fine-structure corrections are identical between the bracketed pairs ($2s_{1/2}$, $2p_{1/2}$), ($3s_{1/2}$, $3p_{1/2}$) and ($3p_{3/2}$, $3d_{3/2}$), thereby making the corresponding total energies the same. On the other hand, the introduction of screening has the following influences on the fine-structure correction: (i) a suppression in magnitude of the fine-structure correction is noticed for each (nlj) fine-structure level with increasing screening strength, and (ii) as the screening is switched on, an l-dependence is introduced in the fine-structure correction, which becomes more pronounced with stronger screening. This is manifested in Table 1 in the increasing difference of the fine-structure correction between the aforementioned pairs of levels with larger non-zero values of μ, and also from Figures 2a and 2b where we have shown the magnitude suppression of the fine-structure correction with increasing screening strength for the $n = 2$ and 3 fine-structure levels in hydrogen. In addition to the magnitude suppression and the lifting of l-degeneracy of the fine-structure correction, now the removal of l-degeneracy of the non-relativistic energy levels splits a non-relativistic level with principal quantum number n into $(2n - 1)$ number of multiplet components for a screened Coulomb atom, in contrast with n number of such fine-structure levels in a normal Coulomb atom (we refer to the last paragraph of this section and Fig. 5 for this deformation in the multiplet structure). In Table 1, we have compared the perturbatively-obtained fine-structure corrections ΔE^{PERT} against the calculated "exact" values $\Delta E^{\mathrm{EXACT}}$; little discrepancies are seen to crop up as the screening strength becomes high for a particular level, but the screening-dependent behavior of ΔE^{PERT} as already discussed is qualitatively preserved by $\Delta E^{\mathrm{EXACT}}$ very well.

A noteworthy feature would be the emergence of the fine-structure correction as a factor of growing importance (despite its suppression) in the total binding energy of the atom as the charges within the screened Coulomb atom faces stringent screening conditions. This is discussed with reference to the ground state $1s_{1/2}$ of hydrogen and is depicted in Figure 3. At no screening the percentage of binding explained by the fine-structure correction in this state, *i.e.* the quantity $100|\Delta E^{\mathrm{PERT}}|/[|E^{\mathrm{NR}}| + |\Delta E^{\mathrm{PERT}}|]$ is as low as 0.001 33% of the total binding energy (the denominator above). With increasing μ, the fine-structure contribution rapidly increases by about two orders of magnitudes in the vicinity of $\mu = 1$ to become quite a sizable proportion $\sim$ 1.215% of the total binding at $\mu = 1.18$ (this is because the % reduction of the non-relativistic binding with screening is much faster than that of the fine-structure correction). Perhaps, even at

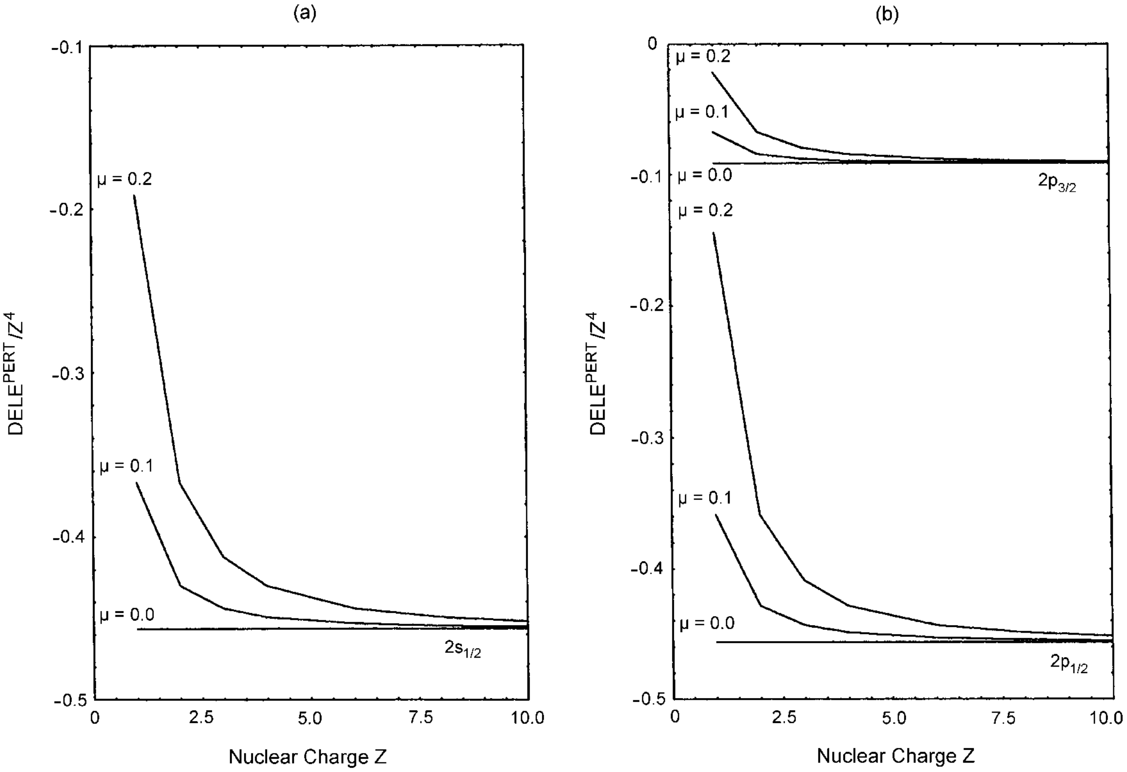

Fig. 4. Departure of the fine-structure correction (ΔE^{PERT}) from its Z^4-scaling for free ($\mu = 0$) hydrogen-like ions in the cases of screened Coulomb ions with $\mu = 0.1$ and 0.2: (a) the $2s_{1/2}$ level, and (b) the $2p_{1/2}$ and $2p_{3/2}$ levels.

this point the validity of a perturbative treatment of the fine-structure correction may be assumed; however, it is to be pointed out that the onset of the non-perturbative regime is nearby and, whether the magnitude of the fine-structure correction $|\Delta E^{\mathrm{PERT}}|$ might eventually become comparable to, or even larger than the non-relativistic binding energy $|E^{\mathrm{NR}}|$ under still stronger screening would be an interesting question for which a non-perturbative analysis of the fine-structure in this region is mandatory. A simultaneous calculation of the "exact" fine-structure correction and its contribution to the "exact" total binding, *i.e.* the quantity $100|\Delta E^{\mathrm{EXACT}}|/|E^{\mathrm{DIRAC}}|$ (where, $|E^{\mathrm{DIRAC}}| = |E^{\mathrm{NR}}| + |\Delta E^{\mathrm{EXACT}}|$), which is also shown in Figure 3 for comparison, supports the foregoing view regarding the importance of fine-structure contribution under stronger screening – this "exact" relativistic contribution to binding exhibits a behavior similar to the "perturbative" one and attains ~ 2.8% of the total binding at $\mu = 1.19$. This describes the "microwave ionization" regime in hydrogen (binding energy ~ 0.03–10 cm^{-1}), where the electron is in the close vicinity of the continuum and is extremely loosely bound to the nucleus such that the ground state $1s_{1/2}$ is only *quasi-stable*. Our calculation hints at the possibility of having a binding in this region which is more of a "relativistic" origin than being essentially of a non-relativistic character.

The trend of variation of the fine-structure correction with nuclear charge Z of larger ions along the hydrogen isoelectronic sequence is the next aspect to be explored. For this purpose we have computed the fine-structure corrections for H-like one-electron positive ions He$^+$, Li^{2+}, Be^{3+}, C^{5+}, O^{7+}, Ne^{9+} with $Z = 2, 3, 4, 6, 8, 10$ respectively at the screening strength values $\mu = 0$, 0.1 and 0.2. The results are displayed graphically in Figures 4a and 4b for the $2s_{1/2}$ and ($2p_{1/2}$, $2p_{3/2}$) levels respectively. For the zero-screening case in Coulomb ions, it follows from equation (7d) that for a particular (nlj)-level $\Delta E^{\mathrm{PERT}} = const \times Z^4$, so that the ratio $\Delta E^{\mathrm{PERT}}/Z^4$ is a constant, independent of Z. This is represented by the horizontal straight lines corresponding to $\mu = 0$ in the graphs where the constants are given by -0.4565 for the $2s_{1/2}$ and by (-0.4565, -0.0913) for the ($2p_{1/2}$, $2p_{3/2}$) levels (see Tab. 1). On the contrary, for screened Coulomb ions with $\mu = 0.1$ and 0.2 quite conspicuous deviations from the Z^4-scaling of ΔE^{PERT} are observed as the ratio is now seen to depend on Z and μ both, exhibiting a non-linear behavior. For an ion with nuclear charge Z, increasing departure from the straight line is obtained with larger screening strengths, and at a particular screening strength the departure is more prominent for lower-Z ions as its electron cloud is less rigidly bound to the nucleus and hence, more responsive to the screening effects than in the relatively immune higher-Z cases.

Finally, the screening-induced deformation of atomic multiplets is illustrated by means of the energy-level diagrams of Figure 5, referring to the $n = 2$ state of hydrogen at no-screening condition $\mu = 0$, and at a screening strength $\mu = 0.2$. The diagrams are self-explanatory – for the Debye-screened atom we notice

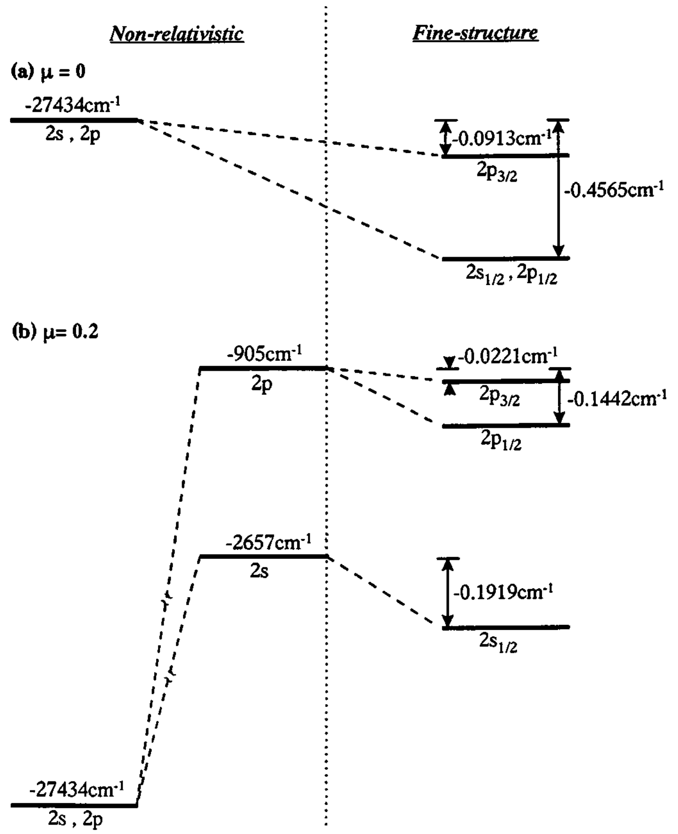

Fig. 5. The deformation of the $n = 2$ fine-structure multiplet of hydrogen in the presence of screening: (a) normal multiplet structure for a free Coulomb atom ($\mu = 0$); (b) distorted multiplet structure for a screened Coulomb atom ($\mu = 0.2$), (the diagrams are only schematic, and are *not to scale*).

the appearance of three multiplet members instead of the two for a Coulomb atom, with a large energy difference between the two extremes of them. While this difference is chiefly an outcome of screening at the non-relativistic level of calculation, the additional level is due to the same at the relativistic level. We may point out in this context that, similar observations should be reflected in the fine-structure emission multiplets of impurity lines in a dense plasma (where more appropriate screening models must be used), and for an actual analysis of the inter- and intra-multiplet transitions for plasma diagnostic purposes, such a distorted multiplet should be the right one that need to be taken into account in lieu of the normal multiplet structures of the isolated (*i.e.*, vacuum-embedded) Coulomb atom.

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