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Variational calculations for the energy levels of confined two-electron atomic systems

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Abstract. An accurate variational calculation has been performed for the ground-state-energy values of confined two-electron isoelectronic series from He to Ar^{16+}. The confinement is obtained by embedding the ion in an overall charge neutral environment like that of a plasma. The confinement potential is chosen as that of a screened Coulomb potential between charges, obtained from a Debye model. The wave function is expanded in terms of product basis sets involving interparticle coordinates. The energy levels are found to be less bound with an increase of the screening parameter and ultimately become unstable. One- and two-particle moments have been calculated for the first time under such screening. The study is expected to throw new light on the behavior of the energy levels of foreign atoms embedded in an overall neutral environment which can be treated like a plasma.

Key words: Confined atoms – Variational calculations – Debye plasma

1 Introduction

Recent advancements in experimental investigations on the spectral line shifts of foreign atoms in liquid helium environments [1, 2, 3, 4, 5, 6, 7] and their interpretations [8, 9] have opened up challenging areas for accurate theoretical estimations of the shift of energy levels of foreign atoms and associated spectral properties under spatial confinement. From a basic theoretical point of view, the confinement of a foreign atom is created by the presence of neighbouring atoms producing an altered potential at the electronic charge cloud of the foreign atom. Thus, in effect, one has to solve the energy eigenvalue problem due to an altered Hamiltonian incorporating the interactions with neighbouring atoms. Although a number of theoretical investigations on varieties of model quantum confining potentials have been performed, revealing a wealth of information for the so-called quantum dots and artificial atoms [8, 9, 10, 11, 12, 13] (see the reviews in Refs. [14, 15]), most of them are concerned with one-electron problems or an effective one-electron problem [16, 17, 18, 19, 20] and ignore electronic correlation effects. In this regard Ludena and Gregory [21] performed configuration interaction calculations on the energy levels of two-electron atoms in a spherical box. Very recently Bieliñska-Wąż et al. [22] have analysed in detail the energy levels of two-electron quantum dots under a quadratic confinement potential which takes care of the effect of electron correlation and they obtained interesting behaviour of the energy levels under various confining potential strengths.

The present communication reports the behaviour of the ground-state energy levels of two-electron atomic systems and other properties under a confining potential created by an overall charge neutral environment which is akin to that created by the presence of liquid helium embedding a foreign atom or that obtained in a nanocavity surrounding a foreign atom. The treatment should be a quantum chemical many-body calculation involving multiple confining centres, which is, by and large, very complicated. Alternatively, one can use a model potential due to the environment atoms and make a rigorous calculation including full correlation under such a model potential. We have considered the model potential due to the overall background of neutral atoms as that created due to a plasma. This is because the foreign atom is embedded by a cluster of helium atoms, the mobility of the electronic charge cloud of which is pretty large [9] and as a result one can treat the foreign atom as being embedded in a plasma environment. From classical electrostatics, the effect of the plasma is to produce an effective screening of the Coulomb potential between two charges. This screened Coulomb potential, originally due to Debye, was introduced in the Hamiltonian and the energy eigenvalues were estimated for the ground state only, including electron correlation effects.

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The model potential has its application in plasma physics [23] and has recently been applied for the study of the electron affinity of hydrogen [24] and in a time-dependent variational calculation for the energy levels of helium-like carbon ion [25]. Lam and Varshni [26] performed correlated calculations on the ionisation energy of the He atom in a Debye plasma. The overall effect of this screened Coulomb potential is to reduce the binding energy and to push the system towards gradual instability with an increase of screening. Actually the screening constant is a function of the temperature and the number density of the plasma and as such different plasma conditions can be simulated by changing the screening parameters. The experimental feasibility of generating laser-produced and tokamak plasmas necessitates the understanding of the electronic spectrum of an ion as a function of the electron density and the temperature of the plasma. The effect of screening is important in different areas of physics, for example, the disappearance of spectral lines near the series limit in astrophysical observations, in plasma diagnostics and in calculating partition functions in thermodynamics, in the calculation of collisional rate coefficients and in semiconductor physics, all of which require the shifted energy levels and properties connected with them. Such conditions are physically obtained in astrophysical, laser-produced or laboratory tokamak plasmas. We performed elaborate calculations on the effect of such screening on the ground-state-energy values of a number of two-electron ions from He to Ar^{16+} taking full care of electron correlations. The method adopted for the calculations is briefly described in Sect. 2 and the results are discussed in Sect. 3.

2 Method

We consider here a two-electron atomic system with nuclear charge $\boldsymbol{Z}$. The nonrelativistic Hamiltonian for the free atom is given by (atomic units are used throughout)

$$H_0 = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z}{r_1} - \frac{Z}{r_2} + \frac{1}{r_{12}}. \tag{1}$$

The energy levels of the free atom can be obtained by solving the usual Schrödinger equation:

$$H_0\Psi = E_0\Psi. \tag{2}$$

With an overall neutral background which mimics a plasma surrounding the atomic system, the electrostatic interaction between any two charges is modified from Coulomb to screened Coulomb (Yukawa) type [23]. The modified Hamiltonian is given by

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{Z\mathrm{e}^{-\mu r_1}}{r_1} - \frac{Z\mathrm{e}^{-\mu r_2}}{r_2} + \frac{\mathrm{e}^{-\mu r_{12}}}{r_{12}}, \tag{3}$$

where μ is a screening constant called the Debye screening parameter arising from the shielding effect due to the surrounding plasma and is given by

$$\mu = \sqrt{\frac{4\pi(1+Z)n}{kT}}. \tag{4}$$

Here n is the number density of electrons in the plasma and the other quantities have their usual significance [23]. A large number of plasma conditions can be simulated by suitably changing the values of the number density and the temperature of the plasma. This is accounted for in our model calculation by suitably changing the values of μ from a very low value to a value where the system becomes unstable.

Our aim is to find the solution of the Schrödinger equation

$$H\Phi = E\Phi \tag{5}$$

using a variational technique. We assume a correlated description of the ground-state (^{1}S) wave function involving interparticle coordinates in its expansion in terms of suitable product basis functions and write its spatial part as

$$\Phi(1,2) = \sum_{ij} C_{ij}\chi_i(1,2)\eta_j(1,2), \tag{6}$$

where $\chi_i(1, 2)$ is a product basis given by

$$\chi_i(1,2) \sim \xi_k(1)\xi_l(2) + \xi_k(2)\xi_l(1), \tag{7}$$

where the ξ_ks are suitable Slater-type orbitals (STO) of the form

$$\xi_k(r) \sim r^{n_k}\mathrm{e}^{-\rho_k r} \tag{8}$$

and in general the term η_j contains the interparticle coordinate:

$$\eta_j(1,2) \sim r_{12}^{mj}. \tag{9}$$

The wave function described by Eq. (8) satisfies the Pauli principle, as the spin part, not shown here, is antisymmetric. For the ^{1}S ground state studied here, the entire problem may be recast in terms of the independent variables r_1, r_2 and r_{12} [27] with suitable averaging over the angular part which is spherically symmetric and the energy eigenvalue is obtained from the lowest root of the generalized eigenvalue equation:

$$\underline{\underline{H}}\underline{C} = E\underline{\underline{S}}\underline{C}, \tag{10}$$

where $\underline{\underline{H}}$ and $\underline{\underline{S}}$ are, respectively, the Hamiltonian and the overlap matrices with respect to the basis given by Eq. (6). Equation (10) is solved for different values of the screening constants μ. For He we chose a five-parameter optimized STO representation for the χ_is (Eq. 8) obtained from Clementi and Roetti [28]. This choice results in a 15-parameter representation for the product set in the expansion of χ_i (Eq. 7). With this radially correlated set we used a five-parameter representation for η_j given by the values of m as $0, 1, \ldots, 4$. Thus, the number of independent coefficients becomes $15 \times 5 = 75$. For all other ions from Li^+ to Ar^{16+}, the number of STO parameters is chosen as 4 of which three are the optimized set of Clementi and Roetti [28]. These are augmented by one extra STO parameter having a relatively smaller value. This parameter is properly optimised to incorporate the diffuseness of the atomic orbital due to larger screening. We did not optimise the nonlinear parameters of the basis for each Debye parameter but the extended nature of the basis is assumed to be adequate to represent the qualitative behaviour of the properties correctly for larger screening. For the angular correlated part of the expansion the number of parameters is 5 throughout, resulting in 50 independent linear variational coefficients in the expansion of the two-particle wave function. The coefficients and the ground-state-energy values were obtained for different screening parameters corresponding to different plasma strengths or different confinement strengths. The results are discussed in Sect. 3.

3 Results and discussion

The nonrelativistic ground-state-energy values for the two-electron ions from He to Ar^{16+} under a screened Coulomb potential were calculated with the view to understand the behaviour of the confined energy levels under an overall neutral environment. Different values of the screening parameters, ranging from zero (no screening) to an upper limit determined by the stability of the system, were incorporated as it was found that with increase of screening the energy values become less bound. The energy values are listed in Table 1 for all the ions for the case when full screening is taken into

Table 1. Ground-state energy and one- and two-electron moments of He isoelectronic sequence under Debye screening

Ion	μ (au)	$-E$	$\langle 1/r \rangle$	$\langle r \rangle$	$\langle r^2 \rangle$	$\langle 1/r_{12} \rangle$	$\langle r_{12} \rangle$	$\langle r_{12}^2 \rangle$
He	0.00	2.9037162	3.3767	1.8588	2.3861	0.9459	1.4219	2.5158
		2.9037244[a]	3.3766[a]	1.8589[a]	2.3870[a]	0.9458[a]	1.4221[a]	2.5164[a]
	0.01	2.8738306	3.3568	1.8588	2.3863	0.9359	1.4220	2.5159
	0.01	2.87255[b]						
	0.50	1.6552679	2.4385	1.9726	2.7304	0.5400	1.5104	2.8608
	0.50	1.65253[b]						
	1.00	0.8159995	1.6322	2.2932	3.7827	0.2751	1.7643	3.9541
	1.00	0.80851[b]						
	2.00	−0.012209	0.5365	3.5116	8.5749	0.0454	2.8007	9.9393
	2.00	0.0063[b]						
Li^{+}	0.00	7.2798191	5.3754	1.1460	0.8935	1.5675	0.8625	0.9274
		7.2799134[a]	5.3758[a]	1.1455[a]	0.8926[a]	1.5677[a]	0.8623[a]	0.9271[a]
	0.01	7.2299475	5.3554	1.1460	0.8935	1.5575	0.8624	0.9274
	0.10	6.7924170	5.1764	1.1473	0.8959	1.4700	0.8635	0.9298
	1.00	3.3612769	3.5035	1.2554	1.0918	0.7777	0.9481	1.1321
	2.00	1.0911718	1.9888	1.5555	1.7010	0.3150	1.1930	1.8136
	3.00	−0.076012	0.9704	2.0106	2.7783	0.1026	1.6004	3.2567
Be^{2+}	0.00	13.655551	7.3755	0.8286	0.4642	2.1909	0.6188	0.4779
		13.655566[a]	7.3755[a]	0.8294[a]	0.4641[a]	2.1909[a]	0.6188[a]	0.4779[a]
	0.01	13.585686	7.3555	0.8286	0.4642	2.1810	0.6188	0.4779
	0.10	12.968807	7.1760	0.2891	0.4649	2.0926	0.6196	0.4787
	1.00	7.8295851	0.5449	0.8744	0.5233	1.3422	0.6542	0.5378
	2.00	3.8955804	3.7291	1.0040	0.7057	0.7395	0.7562	0.7286
	4.00	−0.0487819	1.3001	1.5173	1.5852	0.1425	1.1959	1.8191
B^{3+}	0.00	22.030875	9.3747	0.6493	0.2842	2.8144	0.4825	0.2909
		22.030970[c]	9.3753[c]	0.6491[c]	0.2839[c]	2.8147[c]	0.4824[c]	0.2908[c]
	0.50	17.855607	8.3853	0.6554	0.2901	2.3459	0.4872	0.2969
	1.00	14.263126	7.4260	0.6718	0.3064	1.9340	0.4999	0.3137
	2.00	8.5425180	5.6302	0.7325	0.3694	1.2562	0.5477	0.3798
	3.00	4.4433146	4.0487	0.8310	0.4805	0.7537	0.6277	0.5029
	5.00	−0.187433	1.7791	1.1252	0.8658	0.2124	0.8885	1.0067
C^{4+}	0.00	32.406070	11.3739	0.5338	0.1917	3.4384	0.3954	0.1954
		32.406245[c]	11.3752[c]	0.5336[c]	0.1915[c]	3.4389[c]	0.3953[c]	0.1954[c]
	0.10	31.319951	11.1742	0.5339	0.1918	3.3395	0.3955	0.1956
	1.00	22.678791	9.4121	0.5466	0.2020	2.5371	0.4054	0.2060
	3.00	9.3165517	5.8845	0.6348	0.2778	1.2273	0.4756	0.2877
	5.00	1.8544507	3.1885	0.8003	0.4423	0.4782	0.6177	0.4889
	6.00	−0.333811	2.2316	0.9060	0.5605	0.2777	0.7159	0.6549
N^{5+}	0.00	44.781141	13.3729	0.4532	0.1380	4.0625	0.3349	0.1403
		44.781444[c]	13.3752[c]	0.4530[c]	0.1378[c]	4.0633[c]	0.3348[c]	0.1402[c]
	0.10	43.495193	13.1731	0.4533	0.1381	3.9634	0.3350	0.1404
	1.00	33.083669	11.4033	0.4611	0.1434	3.1467	0.3411	0.1459
	3.00	16.072851	7.7837	0.5148	0.1814	1.7453	0.3839	0.1868
	5.00	5.4897864	4.8182	0.6144	0.2604	0.8378	0.4679	0.2803
	7.00	−0.561919	2.7054	0.7537	0.3876	0.3479	0.5965	0.4558
O^{6+}	0.00	59.156222	15.3723	0.3974	0.1041	4.6869	0.2905	0.1056
		59.156594[c]	15.3751[c]	0.3935[c]	0.1039[c]	4.6879[c]	0.2904[c]	0.1055[c]
	0.01	59.006365	15.3522	0.3937	0.1041	4.6769	0.2905	0.1056
	0.10	57.670400	15.1724	0.3938	0.1041	4.5877	0.2905	0.1056
	1.00	45.481606	13.3970	0.3990	0.1071	3.7602	0.2946	0.1088
	3.00	24.755497	9.7083	0.4347	0.1288	2.2874	0.3230	0.1319
	5.00	10.892866	6.5485	0.5004	0.1723	1.2547	0.3776	0.1821
	8.00	−0.782273	3.1581	0.6493	0.2875	0.4137	0.5139	0.3386
F^{7+}	0.00	75.531401	17.3727	0.3480	0.0812	5.3117	0.2564	0.0823
		75.531712[c]	17.3751[c]	0.3479[c]	0.0811[c]	5.3125[c]	0.2564[c]	0.0823[c]
	0.01	75.361545	17.3527	0.3480	0.0812	5.3017	0.2564	0.0823
	0.10	73.845674	17.1728	0.3481	0.0813	5.2124	0.2565	0.0823
	1.00	59.874815	15.3924	0.3518	0.0832	4.3762	0.2594	0.0843
	2.00	46.605285	13.4753	0.3618	0.0884	3.5580	0.2672	0.0898
	4.00	25.966268	9.9227	0.3981	0.1083	2.2295	0.2963	0.1114
	9.00	−0.8907578	3.5585	0.5769	0.2269	0.4693	0.4557	0.2662
Ne^{8+}	0.00	93.906452	19.3723	0.3119	0.0652	5.9363	0.2295	0.0659
		93.906802[c]	19.3751[c]	0.3117[c]	0.0651[c]	5.9372[c]	0.2295[c]	0.0659[c]
	0.01	93.716596	19.3523	0.3119	0.0652	5.9263	0.2295	0.0660
	1.00	76.264547	17.3891	0.3146	0.0664	4.9942	0.2317	0.0673

Table 1. (continued)

Ion	μ (au)	$-E$	$<1/r>$	$<r>$	$<r^2>$	$<1/r_{12}>$	$<r_{12}>$	$<r_{12}^2>$
	5.00	27.223299	10.1862	0.3671	0.0923	2.2017	0.2739	0.0954
	8.00	6.9726818	6.0265	0.4456	0.1364	0.9916	0.3418	0.1499
	10.0	−1.154708	4.0117	0.5135	0.1796	0.5356	0.4055	0.2109
Na^{9+}	0.00	114.28165	21.3731	0.2825	0.0534	6.5613	0.2077	0.0540
		114.28188^{c}	21.3751^{c}	0.2824^{c}	0.0534^{c}	6.5620^{c}	0.2077^{c}	0.0540^{c}
	0.10	112.19606	21.1732	0.2825	0.0535	6.4619	0.2077	0.0540
	1.00	94.651808	19.3867	0.2845	0.0543	5.6134	0.2093	0.0549
	4.00	49.499513	13.7621	0.3105	0.0656	3.3143	0.2298	0.0668
	8.00	13.377533	7.5873	0.3868	0.1031	1.3436	0.2935	0.1105
	11.0	−1.1319685	4.3672	0.4712	0.1511	0.5820	0.3710	0.1763
Mg^{10+}	0.00	136.65672	23.3732	0.2582	0.0446	7.1862	0.1897	0.0451
		136.65694^{c}	23.3751^{c}	0.2581^{c}	0.0446^{c}	7.1868^{c}	0.1897^{c}	0.0455^{c}
	0.10	134.37118	23.1733	0.2582	0.0446	7.0867	0.1897	0.0451
	1.00	115.03709	21.3848	0.2598	0.0452	6.2337	0.1910	0.0457
	4.00	64.183923	15.7098	0.2799	0.0532	3.8780	0.2068	0.0540
	8.00	21.421294	9.2832	0.3390	0.0791	1.7488	0.2555	0.0836
	12.0	−1.2948599	4.7821	0.4308	0.1263	0.6406	0.3389	0.1471
Al^{11+}	0.00	161.03180	25.3734	0.2377	0.0378	7.8111	0.1746	0.0382
		161.0190^{d}	25.375^{d}	0.2366^{d}	0.0374^{d}	7.8416^{d}	0.1735^{d}	0.0376^{d}
	0.10	158.54631	25.1734	0.2377	0.0378	7.7115	0.1746	0.0382
	1.00	137.42088	23.3833	0.2390	0.0383	6.8547	0.1756	0.0386
	4.00	80.830182	17.6664	0.2549	0.0440	4.4504	0.1881	0.0447
	8.00	31.269331	11.0327	0.3019	0.0627	2.1840	0.2264	0.0655
	13.0	−1.408049	5.1823	0.3978	0.1077	0.6961	0.3125	0.1251
Si^{12+}	0.00	187.40687	27.3734	0.2202	0.0325	8.4360	0.1617	0.0327
		187.3941^{d}	27.3756^{d}	0.2192^{d}	0.0320^{d}	8.4666^{d}	0.1607^{d}	0.0323^{d}
	0.10	184.72140	27.1735	0.2202	0.0325	8.3364	0.1617	0.0327
	1.00	161.80347	25.3821	0.2213	0.0328	7.4763	0.1625	0.0331
	4.00	99.443822	19.6318	0.2342	0.0371	5.0306	0.1725	0.0376
	8.00	42.940599	12.8336	0.2720	0.0508	2.6467	0.2031	0.0527
	10.0	23.674964	9.9688	0.2997	0.0619	1.8060	0.2266	0.0659
	14.0	−1.5406846	5.5863	0.3692	0.0927	0.7524	0.2899	0.1076
P^{13+}	0.00	215.78191	29.3735	0.2052	0.0282	9.0609	0.1506	0.0284
	0.10	212.89649	29.1735	0.2052	0.0282	8.9612	0.1506	0.0284
	1.00	188.18508	27.3812	0.2060	0.0284	8.0984	0.1512	0.0286
	4.00	120.03058	21.6039	0.2166	0.0317	5.6169	0.1594	0.0320
	8.00	56.468339	14.6733	0.2474	0.0420	3.1318	0.1842	0.0433
	12.0	16.700352	9.0820	0.2972	0.0608	1.5160	0.2267	0.0660
	15.0	−1.6992228	5.9951	0.3443	0.0806	0.8098	0.2701	0.0934
S^{14+}	0.00	246.15697	31.3736	0.1920	0.0247	9.6858	0.1409	0.0248
	1.00	216.56591	29.3805	0.1927	0.0249	8.7209	0.1414	0.0250
	4.00	142.59595	23.5793	0.2015	0.0274	6.2076	0.1482	0.0277
	8.00	71.890273	16.5344	0.2271	0.0353	3.6321	0.1686	0.0362
	10.0	46.245436	13.4287	0.2460	0.0417	2.6542	0.1842	0.0435
	14.0	10.210540	8.3288	0.2947	0.05959	1.2883	0.2268	0.0661
	16.0	−1.7845753	6.3877	0.3232	0.0710	0.8637	0.2533	0.0821
Cl^{15+}	0.00	278.53201	33.3737	0.1805	0.0218	10.3107	0.1323	0.0219
	0.10	275.24663	33.1737	0.1805	0.0218	10.2110	0.1323	0.0219
	1.00	246.94608	31.3798	0.1811	0.0219	9.3437	0.1328	0.0221
	4.00	167.14190	25.5596	0.1884	0.0239	6.8026	0.1385	0.0242
	8.00	89.205294	18.4239	0.2098	0.0301	4.1491	0.1555	0.0308
	10.0	60.245752	15.2290	0.2256	0.0350	3.1146	0.1684	0.0363
	17.0	−1.9593570	6.7983	0.3039	0.0628	0.9214	0.2381	0.0726
Ar^{16+}	0.00	312.90704	35.3737	0.1702	0.0194	10.9357	0.1248	0.0195
	0.10	309.42168	35.1738	0.1702	0.0194	10.8360	0.1248	0.0195
	1.00	279.32569	33.3792	0.1707	0.0195	9.9667	0.1252	0.0196
	4.00	193.67196	27.5424	0.1770	0.0211	7.4008	0.1300	0.0213
	8.00	108.44023	20.3280	0.1950	0.0260	4.6772	0.1443	0.0265
	12.0	49.610085	14.0718	0.2246	0.0347	2.6879	0.1687	0.0365
	18.0	−2.1020913	7.2023	0.2869	0.0560	0.9778	0.2248	0.0646

[a] Reference [29] [b] Reference [26] [c] Reference [30] [d] Reference [31]

consideration. To see the behavior of other ground-state properties, we calculated the one- and two-electron moments, such as $<1/r>$, $<r>$, $<r^2>$, $<1/r_{12}>$, $<r_{12}>$ and $<r_{12}^2>$ for all ions with different Debye parameters. The present calculation is highly correlated. This can be found from a comparison of the energy values and the one- and two-electron moments for the free-ion case with the accurate multiterm variational estimates of Drake [29] and Thakkar and Smith [30]. The multiterm variational results, the best available in the literature, were truncated appropriately for comparison purposes wherever necessary. It is observed from Table 1 that both the energy and the moment values agree to a high degree of accuracy up to Mg^{10+}. The present results for He with a Debye parameter greater than zero compare very well with the only data of Lam and Varshni [26]. For Al^{11+} and Si^{12+} multiterm variational results, to our knowledge, are not available and we compared our results with those of Roy and Talukdar [31], which are comparatively less accurate. This is the reason for the apparent deviation of the structural parameters listed in Table 1 for such ions. With an increase of screening the energies become positive, resulting in instability. However, we observe no abrupt change in the expectation value of the one- and two-particle moment operators, but instead smooth behaviour when the energy values become positive. The pattern is consistent for all the ions under study. To see the overall behaviour of the energy values we plotted in Fig. 1 the scaled energy ($-E/Z^2$) against the screening parameter for all the ions. Very regular behaviour is observed for each ion. It is noted that the energy becomes positive at a Debye parameter close to the nuclear charge of a particular ion. Plots of the one- and two-particle moments against the screening parameter for He are shown in Figs. 2 and 3. While the moments $<1/r>$ and $<1/r_{12}>$ decrease continuously with respect to μ, those of $<r>$, $<r^2>$, $<r_{12}>$ and $<r_{12}^2>$ increase as expected. A similar pattern is observed numerically for all the other ions. With an increase of the screening parameter it is observed that the absolute values of the kinetic and potential energies diminish but the potential energy diminishes at a faster rate than the kinetic energy. This produces gradual instability in the system and

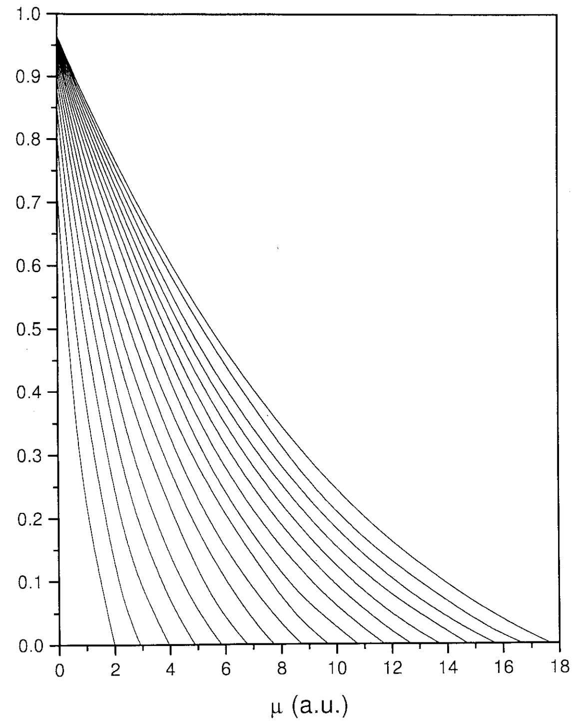

Fig. 1. Scaled ground state energy ($-E/Z^2$) against Debye parameter, μ, for all ions. The *lowermost curve* is for He and the *uppermost curve* is for Ar^{16+}

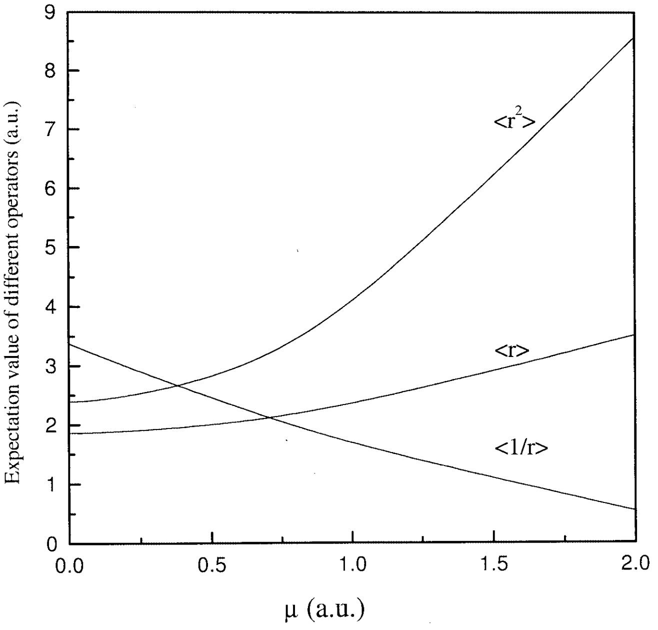

Fig. 2. One-electron moments with μ for He

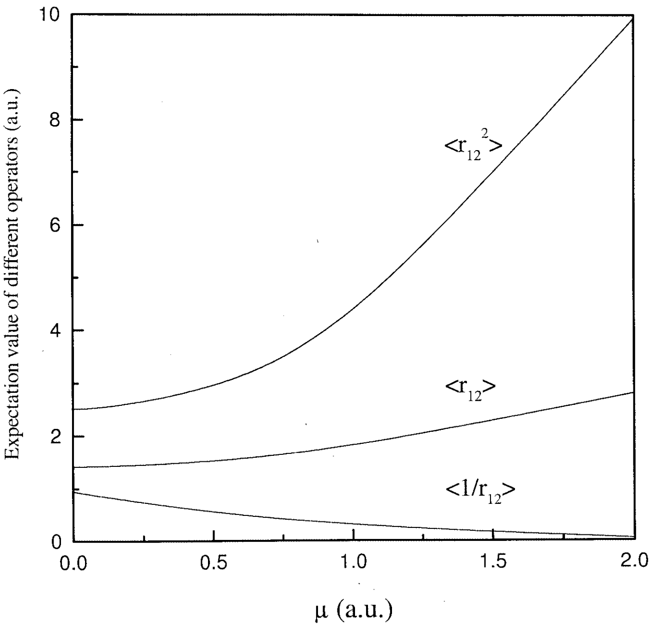

Fig. 3. Two-electron moments with μ for He

deviation of the virial ratio from its free ionic value. The virial ratio, however, is not displayed in the table.

The aim of the present study is to make accurate estimates of energy and other properties of the ground states of He-like ions using the Debye screening model. Experimental results for the properties of the ions studied here are not available and a comparison is made with the very few available theoretical estimates of Lam and Varshni [26] for He only. To make an actual comparison with the available experimental data for the spectral line shifts for multielectron atoms one has to make similar calculations for the ground as well as the excited states of those systems. Such studies for ions for which precise experimental data for the energy level shifts are available are currently in progress. This may give new insight into the behaviour of the spectra of foreign atoms under liquid helium or of nanoconfinements where the central atom is inside a charged neutral environment along with some spatial confinement.

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