Ground state of the lithium atom in strong magnetic fields

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The ground and some excited states of the Li atom in external uniform magnetic fields are calculated by means of our two-dimensional mesh Hartree-Fock method for field strengths ranging from zero up to 2.35×10^8 T. With increasing field strength, the ground state undergoes two transitions involving three different electronic configurations: for weak fields, the ground-state configuration arises from the field-free $1s^2 2s$ configuration; for intermediate fields, it arises from the $1s^2 2p_{-1}$ configuration, and in high fields, the $1s 2p_{-1} 3d_{-2}$ electronic configuration is responsible for the properties of the atom. The transition field strengths are determined. Calculations on the ground state of the Li^+ ion allow us to describe the field-dependent ionization energy of the Li atom. Some general arguments on the ground states of multielectron atoms in strong magnetic fields are provided.
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I. INTRODUCTION

The behavior and properties of atoms in strong magnetic fields is a subject of increasing interest. On the one hand, this is motivated by the astrophysical discovery of strong fields on white dwarfs and neutron stars [1–3], and, on the other hand, the competition of the diamagnetic and Coulombic interaction causes a rich variety of complex properties which are of interest on their own. Investigations of the electronic structure in the presence of a magnetic field appear to be quite complicated due to the mixed geometry of this quantum problem (mixing of spherical and cylindrical symmetries). There are many works on the hydrogen atom (for a list of references, see Refs. [4–7]), and several works on the He atom as well as He-like ions [8–12]. Other atoms, however, have been investigated only in a very few cases [11,13,14].

For the hydrogen atom the impact of the mixed symmetry is particularly evident, and at the same time pronounced in the intermediate-field regime for which the magnetic and Coulomb forces are comparable. For different electronic degrees of excitation of the atom, the intermediate regime is met for different absolute values of the field strength. For the ground state the boundaries of this regime can be defined in a rough manner as the range $\gamma = 0.2$–20 ($\gamma = B/B_0$, B is the magnetic-field strength, $B_0 = \hbar c/e a_0^2 = 2.3505 \times 10^5$ T; a.u. will be used in the following). With increasing degree of excitation the domain of the intermediate fields lowers correspondingly and becomes, as a rule, wider on a logarithmic scale of γ. Both early [15] and more recent works [5,16–19] on the hydrogen atom have used different approaches for relatively weak fields (the Coulomb force prevails over the magnetic force), and for very strong fields where the Coulomb force can be considered as weak in comparison with the magnetic forces (adiabatic limit). In early works the Coulomb field was actually considered in this limit as a perturbation for a free electron in a superstrong magnetic field. The motion of an electron parallel to the magnetic field is governed in the adiabatic approximation [20] by a one-dimensional (1D) quasi-Coulomb potential with a parameter, dependent on the magnetic-field strength. The detailed calculations of the hydrogen energy levels carried out by Rösner *et al.* [5] also retained the separation of the magnetic-field strength domains due to a decomposing of the electronic wave function in terms of either spherical (for weak fields) or cylindrical harmonics (for strong fields). A powerful method to obtain comprehensive results on low-lying energy levels in the intermediate regime in particular for the hydrogen atom is provided by mesh methods [6].

For atoms with several electrons the problem of the mixed symmetries is even more intricate than for hydrogen, because different electrons ''feel'' very different Coulomb forces, i.e., possess different single-particle energies, and the domain of the intermediate fields therefore appears to be the sum of the intermediate domains for the separate electrons.

There exist several investigations on two-electron atoms in the literature [8–12,14,21–25]. The majority of them deal with the adiabatic limit in superstrong fields. Most of the early works are Hartree-Fock (HF) calculations for the strong-field domain. There are also several variational calculations for the low-field domain [22,26,27], including calculations by Larsen [22] made at $\gamma \leqslant 2$ for the He atom and at $\gamma \leqslant 5$ for H^-. The latter calculations can be used for evaluations of the correlation energy in the low-field domain. HF calculations [9] are carried out analogously to the approach in Ref. [5], applying two different sets of basis functions to the high- and low-field domains. As a result of the complicated geometry in the intermediate regime, this approach inherently suffers from very slow convergence properties with respect to the energy eigenvalues, and therefore yields only a very low accuracy. Accurate calculations for arbitrary field strengths were carried out in Refs. [8,10] by the 2D mesh HF method. Investigations on the ground state as well as a number of excited states of helium including the correlation en-

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ergy have very recently been performed via a quantum Monte Carlo approach [12]. Very recently, benchmark results with a precision of 10^{-4}–10^{-6} for the energy levels have been obtained for a large number of excited states with different symmetries using a configuration interaction approach with an anisotropic Gaussian basis set [28].

For the lithium atom, which is the subject of the present work, there exists only one recent investigation in Ref. [11]. It contains calculations for the ground state and a few low-lying states of the Li atom at weak and intermediate fields. Precise Hartree-Fock results for several states in weak fields, and quite satisfactory results for the intermediate region, are presented in this work. However, their basis functions did not allow the authors to perform calculations for stronger fields. An attempt to define the sequence of the electronic ground-state configurations which are different for different regimes of the field strength has also been undertaken in this work. However, a detailed qualitative analysis of the high-field ground-state configuration was not carried out. As a result, the high-field ground-state electronic configuration and the transition point to this configuration from the intermediate one is still an open question.

In the current work we apply a fully numerical 2D Hartree-Fock method to the problem of the Li atom in magnetic fields of arbitrary strength. This method enables us to perform calculations for various states and with approximately equal precision for weak, intermediate, and superstrong magnetic fields. Our main focus is the ground state of the Li atom and its ionization energies. To this end several electronic configurations of the Li atom and two configurations of the Li^+ ion are studied.

II. FORMULATION OF THE PROBLEM AND METHOD OF SOLUTION

We solve the electronic Schrödinger equation for the lithium atom in a magnetic field under the assumption of an infinitely heavy nucleus in the (unrestricted) Hartree-Fock approximation. The solution is established in the cylindrical coordinate system (ρ,ϕ,z), with the z axis oriented along the magnetic field. We prescribe to each electron a definite value of the magnetic quantum number m_μ. Each single-electron wave function Ψ_μ depends on the variables ϕ and (ρ,z)

$$\Psi_\mu(\rho,\phi,z)=(2\pi)^{-1/2}e^{-im_\mu\phi}\psi_\mu(z,\rho), \tag{1}$$

where $\mu=1$, 2, and 3 is the numbering of the electrons. The resulting partial differential equations for $\psi_\mu(z,\rho)$ and the formulas for the Coulomb and exchange potentials were presented in Ref. [10].

The one-particle equations for the wave functions $\psi_\mu(z,\rho)$ are solved by means of the fully numerical mesh method described in Refs. [6,10]. The feature which distinguishes the present calculations from those described in Ref. [10] is the method of calculation of the Coulomb and exchange integrals. In the present work, as well as in Ref. [13], we obtain these potentials as solutions of the corresponding Poisson equations. The problem of the boundary conditions for the Poisson equation, as well as the problem of simultaneously solving Poisson equations on the same meshes with Schrödinger-like equations for the wave functions $\psi_\mu(z,\rho)$, have been discussed in Ref. [10]. In the present approach these problems are solved by using special forms of nonuniform meshes. Solutions to the Poisson equation on separate meshes contain some errors δ_P associated with an inaccurate description of the potential far from the nucleus. However, due to the special form of the function $\delta_P(h)$ for these meshes (where h is a formal mesh step), the errors do not show up in the final results for the energy and other physical quantities, which we obtain by means of the Richardson extrapolation procedure (polynomial extrapolation to $h=0$ [6,29]). An additional improvement with respect to the precision of our numerical calculations of the integrals is achieved by solving the Poisson equation not for the whole charge distribution but for the total distribution minus some properly chosen charge distribution with known analytical solution to the Poisson equation. Both of these approaches will be described in detail in a separate work.

Our mesh approach is flexible enough to yield precise results for arbitrary field strengths. Some minor decrease of the precision appears in very strong magnetic fields. This phenomenon is due to a growing difference in the binding energies $\epsilon_{B\mu}$ of single-electron wave functions belonging to the same electronic configuration

$$\epsilon_{B\mu}=(m_\mu+|m_\mu|+2s_{z\mu}+1)\,\gamma/2-\epsilon_\mu, \tag{2}$$

where ϵ_μ is the single-electron energy and $s_{z\mu}$ is the spin z projection. This results in large differences with respect to the spatial extension of the density distribution for different electrons. This difference is important for the configurations $1s^22s$, $1s2s2p_{-1}$, and $1s2p_02p_{-1}$, and is not important for $1s2p_{-1}3d_{-2}$ and $1s^22p_{-1}$ because all the single-electron energies for the latter states are of the same order of magnitude. The precision of our results depends, of course, on the number of mesh nodes and can be improved in calculations with denser meshes. The most dense meshes which we could use in the present calculations had 120×120 nodes. These meshes were used for the states $1s^22s$, $1s2s2p_{-1}$, and $1s2p_02p_{-1}$ at fields $\gamma=500$ and 1000. For other states and weaker magnetic fields, Richardson's sequences of meshes with a maximal number 80×80 or 60×60 were sufficient.

III. GROUND-STATE ELECTRONIC CONFIGURATIONS

We start this section with a qualitative consideration of the problem of atomic multielectron ground states in the limit of strong magnetic fields. It is clear that the state $1s^22s$ of the lithium atom is the ground state only for relatively weak fields. The set of single-electron wave functions for constructing the HF ground state for the opposite case of extremely strong magnetic fields can be determined as follows. The nuclear attraction energies and HF potentials (which determine the motion along the z axis) are then small compared to the interaction energies with the magnetic field (which determines the motion perpendicular to the magnetic field, and is responsible for the Landau zonal structure of the spectrum). Thus all single-electron wave functions must correspond to the lowest Landau zones, i.e., $m_\mu\leqslant0$ for all the electrons, and the system must be fully spin polarized, i.e., $s_{z\mu}=-\frac{1}{2}$ $(\downarrow)$. For the Coulomb central field the single-electron levels form quasi-1D Coulomb series with the binding energy $E_B=1/2n_z^2$ for $n_z>0$ and $E_B\to\infty$ for $n_z=0$,

where n_z is the number of nodal surfaces of the wave function, which cross the z axis. These relations between single-electron energies and the geometry of single-electron wave functions along with analogous relations for the field-free atom provide the basis for the following considerations.

It is evident that the wave functions with $n_z=0$ have to be chosen for the ground state at $\gamma\to\infty$. Thus for $\gamma\to\infty$ the ground state of the Li atom must be $1s\downarrow 2p_{-1}\downarrow 3d_{-2}\downarrow$. This state was not considered in Ref. [11], but only the $1s\downarrow 2p_0\downarrow 2p_{-1}\downarrow$ configuration was presented. Analogously, the very high-field ground state for the C atom considered in Ref. [11] must be the state belonging to the configuration $1s\downarrow 2p_{-1}\downarrow 3d_{-2}\downarrow 4f_{-3}\downarrow 5g_{-4}\downarrow 6h_{-5}\downarrow$.

The problem of the configuration of the ground state for the intermediate-field region cannot be solved without doing explicit calculations. Calculations in Ref. [11] were carried out for configurations with the maximal single-electron principal quantum number $n\leqslant 2$. Under this restriction calculations for the states $1s^2 2s$, $1s^2 2p_{-1}$, $1s\downarrow 2s\downarrow 2p_{-1}\downarrow$, and $1s\downarrow 2p_0\downarrow 2p_{-1}\downarrow$ are sufficient to determine the set of intermediate ground states. Indeed, $1s^2 2s$ is the zero-field ground state. $1s^2 2p_{-1}$ is the lowest excited state of the field-free atom, and (contrary to $1s^2 2s$) all the single-electron wave functions of this state must have infinite binding energies in the infinite strong magnetic field. Moreover, this state has the largest binding energy E_B,

$$E_B=\sum_{\mu=1}^{3}(m_\mu+|m_\mu|+2s_{z\mu}+1)\,\gamma/2-E, \tag{3}$$

in the strong-field limit due to the fact that $\epsilon_B(1s)>\epsilon_B(2p_{-1})>\epsilon_B(3d_{-2})>\cdots$ in strong fields. [For $\gamma=1000$, one can obtain binding energies from Table I as $E_B(1s^2 2p_{-1})=69.1569$ and $E_B(1s2p_{-1}3d_{-2})=60.0589$]. The reader should note that the $1s^2 2p_{-1}$ configuration cannot represent the ground state in very strong fields, since it is not fully spin polarized. The state $1s\downarrow 2s\downarrow 2p_{-1}\downarrow$ is the lowest fully spin-polarized state with the single-electron principal quantum numbers $n_\mu\leqslant 2$ in weak fields and, at last, the state $1s\downarrow 2p_0\downarrow 2p_{-1}\downarrow$ which lies higher at $\gamma=0$ must become lower than $1s\downarrow 2s\downarrow 2p_{-1}\downarrow$ with increasing field strength.

Our calculations include the high-field ground state $1s\downarrow 2p_{-1}\downarrow 3d_{-2}\downarrow$ which contains one electron with $n=3$. In principle, other configurations could also be considered as possible ground states for intermediate-field strength. Such configurations are $1s^2 3s$, $1s^2 3p_{-1}$, $1s^2 3d_{-2}$, $1s2s3s$, $1s2s3p_{-1}$, $1s2s3d_{-2}$, $1s2p_{-1}3s$, and $1s2p_{-1}3p_{-1}$. Calculations for all these states are possible by means of our mesh HF method. However they are extremely tedious and time consuming, and have not been accomplished in the present work. Indeed, we will argue in the following that none of these states can be the ground state of the Li atom for intermediate-field strength.

It is quite evident that for the configurations containing a $1s^2$ pair of electrons, the $1s^2 3s$ configuration lies higher in energy than the $1s^2 2s$ configuration, and that the $1s^2 3p_{-1}$ and $1s^2 3d_{-2}$ configurations possess higher energy than the $1s^2 2p_{-1}$ configuration. Thus the above-listed states with $1s^2$ pairs can be excluded from our argumentation of the ground state. Among the fully spin-polarized configurations, the levels of the configurations $1s2p_{-1}3s$, $1s2s3p_{-1}$, $1s2s3d_{-2}$, and $1s2p_{-1}3p_{-1}$ are higher than that of the $1s2s2p_{-1}$ configuration (two components of the configurations are identical with those of $1s2s2p_{-1}$ configuration, and the third one is significantly higher). Thus for simple geometrical reasons only the $1s2s3s$ configuration (mixed with the $1s2s3d_0$ configuration) is *a priori* not excluded from becoming the intermediate ground state. In weak magnetic fields this state lies slightly lower than other doubly excited and autoionizing states, and in this regime it is the lowest fully spin-polarized state. But the change of the ground state to the fully spin-polarized configuration takes place in the vicinity of $\gamma=2$, for which the $3s$ wave functions is much more weakly bound than the $3d_{-2}$, $2p_{-1}$, and even $2p_0$ orbitals. Due to this fact the $1s2s3s$ configuration can also be excluded from becoming the ground state for any field strength. Indeed our calculations show that this state becomes higher in energy than the $1s2s2p_{-1}$ state at $\gamma\approx 0.16$. Thus the set $1s^2 2p_{-1}$, $1s\downarrow 2s\downarrow 2p_{-1}\downarrow$, and $1s\downarrow 2p_0\downarrow 2p_{-1}\downarrow$, along with weak-field $1s^2 2s$ and strong-field $1s\downarrow 2p_{-1}\downarrow 3d_{-2}\downarrow$ ground states is comprehensive for a determination of the ground state of the Li atom in a magnetic field of arbitrary strength.

IV. NUMERICAL RESULTS

The only work on the Li atom in a magnetic field with which we can compare our results is Ref. [11]. In this reference, HF calculations were performed for weak and intermediate magnetic-field strengths. Table I contains the total energies obtained for the Li atom within our calculations, in comparison with the data obtained in Ref. [11]. Our energy values coincide with those of Ref. [11] for weak fields, and lie substantially lower in the intermediate regime. At the upper boundary of the field region investigated in Ref. [11] the differences between Ref. [11] and our energies are 0.0239 for the $1s^2 2s$ state, 0.0205 for the $1s^2 2p_{-1}$ state, 0.0870 for the $1s2s2p_{-1}$ state, and 0.0458 for the $1s2p_0 2p_{-1}$ state.

Our results on the total energies are illustrated in Figs. 1 and 2. These figures show, in particular, the ground-state configurations for the different regimes of the field strength. One can conclude from Table I and Figs. 1 and 2 that the $1s^2 2s$ configuration represents the ground state for $0\leqslant\gamma<0.17633$; for $0.17633<\gamma<2.153$, the ground-state configuration is $1s^2 2p_{-1}$; and for $\gamma>2.153$, the ground-state configuration is $1s\downarrow 2p_{-1}\downarrow 3d_{-2}\downarrow$. The state $1s\downarrow 2p_0\downarrow 2p_{-1}\downarrow$ presented in Ref. [11] as the high-field ground state appears not to be the ground state of the Li atom for any magnetic-field strength.

Figure 3 presents spatial distributions of the total electronic densities for the ground-state configurations of the lithium atom. In each row, these densities are presented for the limits of the corresponding field strength regions, including the transition points, and for some value of the intermediate-field strength in between. For each separate configuration the effect of the increasing field strength consists of compressing the electronic distribution toward the z axis. For the $1s2p_{-1}3d_{-2}$ configuration, for which all single-electron binding energies increase unlimitedly for $\gamma\to\infty$, a shrinking process of this distribution in the z direction is also visible. For the $1s^2 2p_{-1}$ configuration this effect

TABLE I. Total energies (in a.u.) of several electronic ground and excited states of the Li atom in the regime of field strength $\gamma = 0, \ldots, 1000$.

	$1s^2 2s$		$1s^2 2p_{-1}$		$1s2s2p_{-1}$		$1s2p_0 2p_{-1}$		$1s2p_{-1}3d_{-2}$
γ	E	E [11]	E	E [11]	E	E [11]	E	E [11]	E
0.0000	−7.432 75	−7.4327	−7.365 09	−7.3651	−5.358 88	−5.3583	−5.231 86	−5.2318	−5.083 79
0.0010	−7.433 26		−7.366 09		−5.360 88		−5.233 86		−5.086 79
0.0018	−7.433 65	−7.4337	−7.366 89	−7.3669	−5.362 47	−5.3625	−5.235 46	−5.2355	−5.089 15
0.0020	−7.433 75		−7.367 09		−5.362 88		−5.235 86		−5.089 76
0.0050	−7.435 22		−7.370 02		−5.368 84		−5.241 82		−5.098 52
0.0090	−7.437 13	−7.4371	−7.373 87	−7.3738	−5.376 73	−5.3767	−5.249 73	−5.2497	−5.109 88
0.0100	−7.437 60		−7.374 81		−5.378 71		−5.251 70		−5.112 68
0.0180	−7.441 25	−7.4412	−7.382 18	−7.3832	−5.394 29	−5.3943	−5.267 34	−5.2673	−5.134 33
0.0200	−7.442 14		−7.383 97		−5.398 17		−5.271 21		−5.139 60
0.0500	−7.453 98		−7.408 44		−5.454 42		−5.327 86		−5.212 81
0.0540	−7.455 37	−7.4553	−7.411 41	−7.4114	−5.461 68	−5.4617	−5.335 21	−5.3352	−5.221 99
0.1000	−7.468 57		−7.441 76		−5.541 49		−5.416 43		−5.321 40
0.1260	−7.474 08	−7.4739	−7.456 50	−7.4565	−5.583 76	−5.5837	−5.459 92	−5.4599	−5.373 71
0.17633	−7.481 62		−7.481 62						
0.1800	−7.482 04	−7.4814	−7.483 30	−7.4832	−5.665 85	−5.6656	−5.545 55	−5.5455	−5.475 68
0.2000	−7.484 00		−7.492 20		−5.694 51		−5.575 85		−5.511 51
0.5000	−7.477 41		−7.587 90		−6.047 87		−5.969 57		−5.970 52
0.5400	−7.473 51	−7.4731	−7.597 09	−7.5965	−6.087 46	−6.0844	−6.016 03	−6.0159	−6.024 14
0.9000	−7.425 04	−7.4240	−7.656 28	−7.6563	−6.401 75	−6.3993	−6.396 13	−6.3956	−6.460 61
1.0000	−7.408 79		−7.666 53		−6.480 29		−6.492 48		−6.570 81
1.2600	−7.362 26	−7.36 09	−7.682 88	−7.6820	−6.674 94	−6.6720	−6.729 31	−6.7284	−6.841 22
1.8000	−7.246 03	−7.2446	−7.676 57	−7.6747	−7.054 30	−7.0403	−7.173 26	−7.1711	−7.347 23
2.0000	−7.196 21		−7.662 46		−7.188 89		−7.324 94		−7.520 03
2.0718 14	−7.177 45		−7.656 00		−7.236 50		−7.377 99		−7.580 47
2.1530			−7.647 85						−7.647 85
2.1600			−7.647 11	−7.6459	−7.294 45	−7.2826	−7.442 18	−7.4404	−7.653 61
2.5000	−7.056 19		−7.603 51		−7.512 55		−7.718 26		−7.925 32
3.0000	−6.895 59		−7.515 16		−7.818 34		−8.008 37		−8.299 20
3.6000	−6.678 74	−6.6640	−7.376 38	−7.3627	−8.163 36	−8.1159	−8.372 14	−8.3564	−8.714 64
3.9600			−7.278 26	−7.2722	−8.359 94	−8.3165	−8.577 39	−8.5578	−8.949 29
4.3200			−7.170 26	−7.1655	−8.549 41	−8.5075	−8.774 15	−8.7526	−9.174 42
4.6800			−7.053 26	−7.0391	−8.732 33	−8.6767	−8.963 27	−8.9371	−9.390 99
5.0000	−6.088 11		−6.942 30		−8.889 81		−9.125 54		−9.576 94
5.0400			−6.928 00	−6.9050	−8.909 18	−8.8375	−9.145 46	−9.1160	−9.599 77
5.4000	−5.901 13	−5.8772	−6.795 17	−6.7747	−9.080 45	−9.0035	−9.321 34	−9.2755	−9.801 47
7.0000	−5.089 09		−6.126 70		−9.783 57		−10.038 96		−10.625 78
10	−3.357 77		−4.617 77		−10.910 59		−11.178 86		−11.939 02
20	3.49120		1.705 65		−13.694 20		−13.965 82		−15.162 60
50	27.6916		24.979 42		−18.8012		−19.04 36		−21.0505
100	71.807		68.1735		−23.987		−24.1946		−27.0192
200	164.371		159.5749		−30.559		−30.7327		−34.5850
500	451.69		444.9033		−41.821		−41.959		−47.5583
1000	939.54		930.843 08		−52.65		−52.771		−60.0589

is not distinct for the relevant field strengths. For the $1s^2 2s$ state the opposite effect can be observed: the $2s$ electronic charge distribution along the z axis expands slightly in weak magnetic fields. A characteristic feature of the transition points is an inflation of the electronic distribution in the ρ direction during transitions from lower- to higher-field ground-state configurations. This effect occurs due to the prevailing of the lowering in energy with changing quantum numbers ($m=0$ to $m=-1$ for the transition point $\gamma = 0.17633$, and $S_z = \Sigma_{\mu=1}^{3} s_{z\mu} = -\frac{1}{2}$ to $S_z = -\frac{3}{2}$ for $\gamma = 2.153$) over the raising of the energy due to more extended charge distributions in the ρ direction.

The total binding energies of the configurations $1s^2 2s$, $1s^2 2p_{-1}$, $1s\downarrow 2s\downarrow 2p_{-1}\downarrow$, $1s\downarrow 2p_0\downarrow 2p_{-1}\downarrow$, and $1s\downarrow 2p_{-1}\downarrow 3d_{-2}\downarrow$ are presented in Fig. 4. These values do not include spin polarization terms, and it can clearly be seen that the atomic ground state in a magnetic field does in general not possess the largest binding energy.

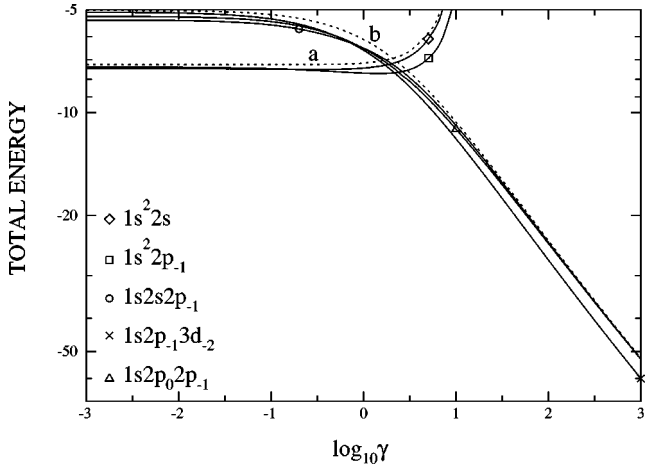

FIG. 1. Total energies (in a.u.) of the Li atom as a function of the magnetic-field strength (solid lines marked by centered symbols). The field strength is given in units of $B_0=\hbar c/ea_0^2=2.3505\times10^5$ T. Dotted lines are energies of two electronic configurations of the Li^+ ion: (a) low-field ground state $1s^2$; (b) high-field ground state $1s2p_{-1}$.

Along with the total energy of the Li-atom ground state, we have obtained its ionization energies E_I dependent on γ. The total-energy values of the ground state of the ion Li^+ are required for these calculations. The set of the ground-state configurations of this two-electron ion is analogous to those of the helium atom [9,10], and consists of the zero-field ground state $1s^2$ and the strong-field fully spin-polarized state $1s\downarrow 2p_{-1}\downarrow$. Results of our calculations for these states are presented in Table II. The change of the ground-state configuration takes place at $\gamma=2.071\,814$. Comparing Tables I and II, one obtains the dependence of the ionization energy of the ground state of the Li atom on the magnetic-field strength, as shown in Fig. 5. This curve exhibits three distinct points marked by dotted vertical lines. The first of them (from left to right) corresponds to the change of the ground-state configuration of the lithium atom from $1s^22s$ to $1s^22p_{-1}$. The second corresponds to the change of the Li^+ ground-state configuration from $1s^2$ to $1s\downarrow 2p_{-1}\downarrow$. And the third, very near to the second one, corresponds to the second change of the Li atom ground-state configuration from $1s^22p_{-1}$ to $1s\downarrow 2p_{-1}\downarrow 3d_{-2}\downarrow$. Table II provides the numerical data for the ionization energies. Tables I and II also allow one to obtain ionization energies for other states presented in Table I.

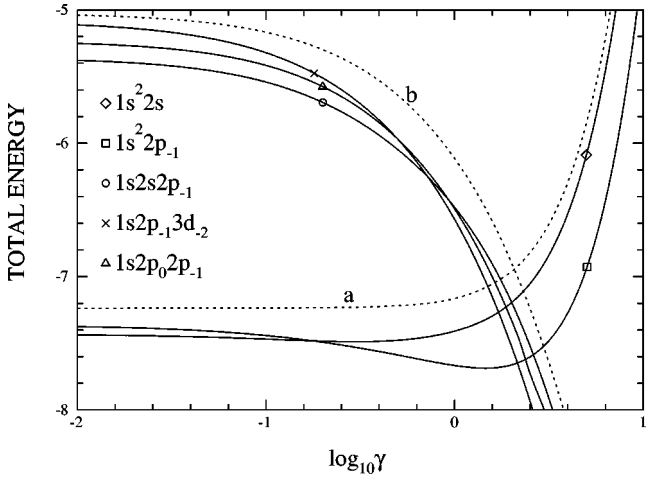

FIG. 2. Total energies (in a.u.) of the Li atom as a function of the magnetic-field strength (solid lines marked by centered symbols) in the relevant regime of transitions of the ground-state configurations. The field strength is given in units of $B_0=\hbar c/ea_0^2=2.3505\times10^5$ T.

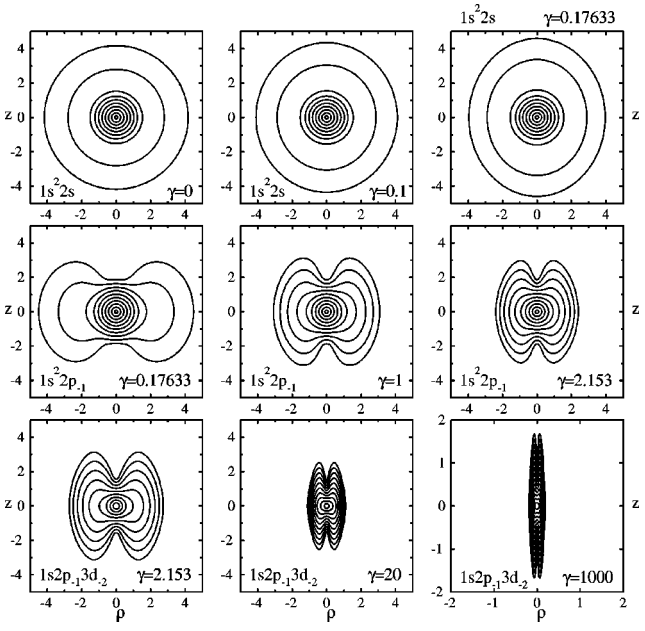

FIG. 3. Contour plots of the total electronic densities for the ground state of the Li atom. The densities for neighbouring lines are different by a factor of e. The coordinates z, and ρ, as well as the corresponding field strengths, are given in a.u.

In addition, in Fig. 6 we show the total quadrupole moment

$$Q_{zz}=\langle\Psi|3z^2-r^2|\Psi\rangle, \quad r^2=\rho^2+z^2 \tag{4}$$

of different states of the atom as a function of the field strength. These dependencies illustrate the changes in the

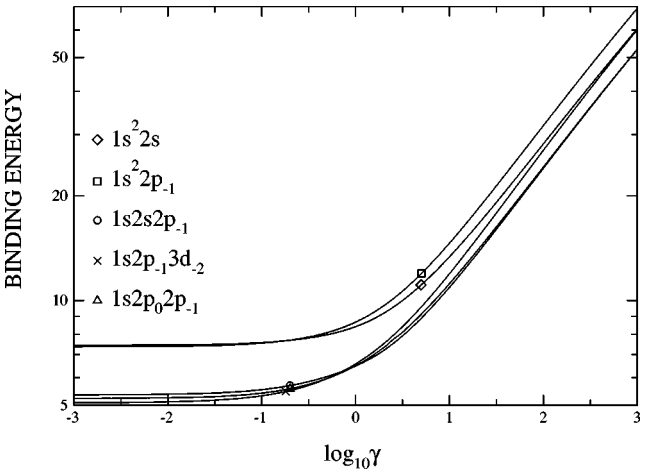

FIG. 4. Binding energies of various states of the Li atom as a function of the magnetic field strength (in atomic units).

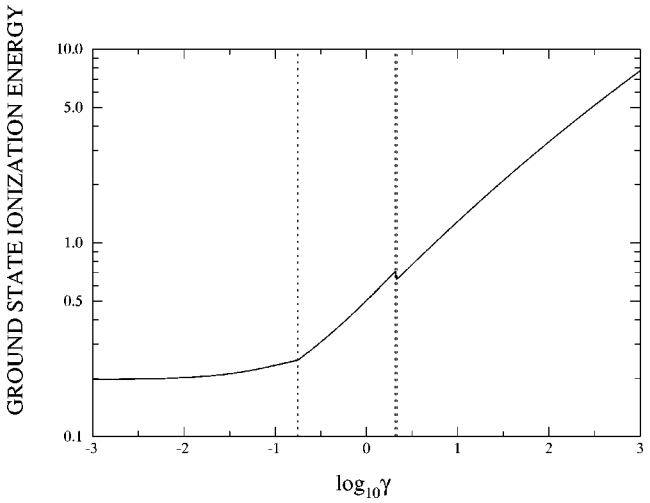

FIG. 5. Li-atom ground-state ionization energy E_I for a broad range of field strengths (in a.u.). Transition points are marked by broken vertical lines. The first transition (from left to right) corresponds to the change of the ground-state configuration from $1s^2 2s$ to $1s^2 2p_{-1}$. The second transition corresponds to the change of the Li^+ ground-state configuration from $1s^2$ to $1s2p_{-1}$. The third transition corresponds to the change of the Li ground-state configuration from $1s^2 2p_{-1}$ to $1s2p_{-1}3d_{-2}$.

TABLE II. Energies (in a.u.) of the low- and high-field ground states of the ion Li^+ and the ionization energy of the ground state of the Li atom E_I for field strengths $\gamma = 0, \ldots, 1000$.

γ	$1s^2$	$1s2p_{-1}$	E_I(Li)
0.0000	−7.236 42	−5.024 69	0.196 33
0.0010	−7.236 42	−5.026 19	0.196 84
0.0020	−7.236 42	−5.027 69	0.197 33
0.0050	−7.236 41	−5.032 18	0.198 81
0.0100	−7.236 41	−5.039 63	0.201 19
0.0200	−7.236 39	−5.054 42	0.205 75
0.0500	−7.236 23	−5.097 97	0.217 75
0.1000	−7.235 67	−5.167 89	0.232 90
0.1763 3	−7.234 11	−5.268 74	0.247 51
0.2000	−7.233 45	−5.298 73	0.258 75
0.5000	−7.217 98	−5.640 06	0.369 92
1.0000	−7.164 01	−6.114 62	0.502 52
2.0000	−6.963 00	−6.894 08	0.699 46
2.0718 14	−6.944 40	−6.944 40	0.711 60
2.1530	−6.922 78	−7.000 57	0.647 29
2.5000	−6.823 47	−7.232 58	0.692 75
3.0000	−6.662 37	−7.546 72	0.752 48
5.0000	−5.850 51	−8.629 43	0.947 51
7.0000	−4.847 25	−9.524 92	1.100 86
10	−3.110 92	−10.651 31	1.287 71
20	3.748 96	−13.429 74	1.732 86
50	27.964 65	−18.525 48	2.5250
100	72.093 37	−23.699 94	3.3193
200	164.668 67	−30.260 77	4.3242
500	452.0032	−41.503 93	6.0544
1000	939.879 76	−52.3230	7.7359

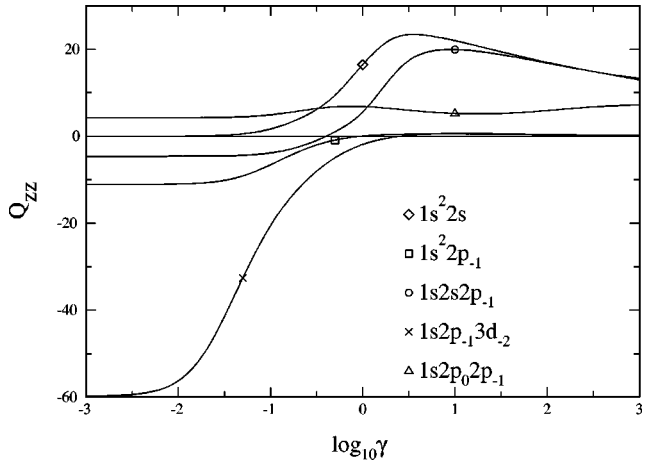

FIG. 6. Quadrupole moment of the Li atom depending on the magnetic-field strength (in a.u.).

density distribution of the electrons with increasing magnetic-field strength. For weak- and, also to some extent, intermediate-field strengths the main effect consists in compressing the wave function toward the z axis. This results in increasing Q_{zz} values and a sign change of Q_{zz} for the states with initially negative Q_{zz}. For $\gamma > 10$ the continuing compression toward the z axis practically does not affect Q_{zz} due to the small values of $\langle \rho^2 \rangle$. The values of Q_{zz} decrease in this region for all states considered, with the exception of the state $1s\downarrow 2p_0\downarrow 2p_{-1}\downarrow$. This decrease of Q_{zz} is associated with the decreasing value of $\langle z^2 \rangle$ due to an increasing one-particle binding energy. For the states $1s^2 2p_{-1}$ and $1s\downarrow 2p_{-1}\downarrow 3d_{-2}\downarrow$, all these binding energies become infinite for infinitely strong fields. This results in $Q_{zz} \to 0$ as $\gamma \to \infty$. For the other states presented in Fig. 6, at least one of the single-electron energies remains finite as $\gamma \to \infty$ and, as a result, Q_{zz} has a finite limit as $\gamma \to \infty$.

Two issues concerning the results presented above have to be discussed. First, our HF results do not include the effects of correlation. To take the latter into account would require a multiconfigurational approach which goes beyond the scope of the present paper. However, we, do not expect that the correlation energy changes our main conclusions, such as, for example, the transitions in the ground-state configurations or the behavior of the ionization energies depending on the field strength. With increasing field strength the effective one-particle picture should be an increasingly better description of the wave function, and the percentage of the correlation energy should therefore decrease.

Additional consideration is required both for the transition points which separate different electronic configurations of the ground state, and for other intersections presented in Figs. 1 and 2. In principle, effects of electronic correlation can turn level crossings into avoided crossings. In this case the classification of the ground state via a single configuration of three single-particle states should break down, and the sharp kinks in Fig. 5 would be smoothed out. But we do not expect these effects of correlation to occur for the ground-state configurations because of the different symmetries of the configurations involved. Indeed, states $1s^2 2s$ and $1s^2 2p_{-1}$ (the first transition point) have different total mag-

netic quantum numbers $M_L=\Sigma_{\mu=1}^{3} m_\mu$, $M_L(1s^2 2s)=0$, and $M_L(1s^2 2p_{-1})=-1$. The third ground-state configuration $1s\downarrow 2p_{-1}\downarrow 3d_{-2}\downarrow$ differs from $1s^2 2p_{-1}$ not only by $M_L(1s\downarrow 2p_{-1}\downarrow 3d_{-2}\downarrow)=-3$ but also by the total spin z projection S_z, $S_z(1s^2 2p_{-1})=-\frac{1}{2}$ and $S_z(1s\downarrow 2p_{-1}\downarrow 3d_{-2}\downarrow)=-\frac{3}{2}$. Analogously the ground-state configurations $1s^2$ and $1s\downarrow 2p_{-1}\downarrow$ of the Li^+ ion have different M_L and S_z. Thus we do not expect that correlation effects can lead to avoided crossings in the ground-state configurations of Li and Li^+. Analogous arguments hold for some of the other intersections presented in Figs. 1 and 2. In particular, the electronic states $1s\downarrow 2s\downarrow 2p_{-1}\downarrow$, $1s\downarrow 2p_0\downarrow 2p_{-1}\downarrow$, and $1s\downarrow 2p_{-1}\downarrow 3d_{-2}\downarrow$ possess a total spin projection S_z different from that of the electronic states $1s^2 2s$ and $1s^2 2p_{-1}$.

The second issue relates to effects of the finite nuclear mass. For the case of hydrogen, it is well known that in the high-field regime ($\gamma \gg 10^2$) mass correction terms due to the finite nuclear mass become relevant, i.e., are no longer negligible in comparison with the Coulomb binding energies. The most important mass, corrections can be included by replacing the electron mass through its reduced mass and results from the infinite nuclear mass calculations are related to those with the reduced mass via a scaling relation. In the case of the much heavier Li atom, these effects are expected to be much smaller.

V. SUMMARY AND CONCLUSIONS

We have applied our 2D mesh Hartree-Fock method to a magnetized Li atom. The method is flexible enough to yield precise results for arbitrary field strengths, and our calculations for the ground and several excited states are performed for magnetic-field strengths ranging from zero up to 2.3505×10^8 T ($\gamma=1000$). Our consideration was focused on the ground state of the Li atom. With increasing field strength this state undergoes two transitions involving three different electronic configurations. For weak fields up to $\gamma = 0.176\,33$, the ground state arises from the field-free $1s^2 2s$ configuration. For intermediate fields ($0.17633<\gamma<2.1530$) the ground state is constituted by the $1s^2 2p_{-1}$ configuration, and for $\gamma>2.1530$ the ground-state configuration is the fully spin-polarized $1s2p_{-1}3d_{-2}$ configuration. We provide arguments which show that this configuration must correspond to the ground state in the strong-field limit. Generalizing these arguments, we could derive the high-field ground-state configuration of arbitrary fully spin-polarized atoms which are constituted by certain tightly bound hydrogenlike states. For example, for atoms with six electrons (i.e., C and C-like ions) the high-field ground state is given by the fully spin-polarized $1s\downarrow 2p_{-1}\downarrow 3d_{-2}\downarrow 4f_{-3}\downarrow 5g_{-4}\downarrow 6h_{-5}\downarrow$ configuration.

We have also calculated HF energies for the two Li^+ ground-state configurations $1s^2$ and $1s\downarrow 2p_{-1}\downarrow$. The first of them forms the ground state at $0\leqslant\gamma<2.071\,814$, the second one is the high-field ground-state configuration for $\gamma>2.071\,814$. These calculations allowed us to obtain the Li atom ground-state ionization energy E_I dependent on the magnetic-field strength. This dependence, opposite to the analogous dependence for the total and binding energies, is not monotoneous, and contains both areas of increasing values of E_I and a domain of decreasing behavior between $\gamma=2.071\,814$ and 2.1530. Furthermore, we have studied the quadrupole moment of the atom and showed how its complicated behavior with changing field strength can be explained through the field dependence of the different HF orbitals.

Apart from the Li atom, other species, i.e., three-electron objects, are expected to be in particular of astrophysical interest: the three-electron ions formed by the nuclei C, O, and Ne possess a high abundance in the universe. To study these systems is the subject of a separate investigation.

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