The 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 2D mesh Hartree-Fock method for field strengths ranging from zero up
to $2.35 \cdot 10^8$ T. With increasing field strength the ground state undergoes two transitions involving
different electronic configurations: for weak fields the ground state configuration arises from
the field-free $1s^22s$ configuration, for intermediate fields from the $1s^22p$ configuration and in high
fields the $1s^22p^23d^2$ 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 multi-electron atoms in strong magnetic fields are provided.

I. INTRODUCTION

The behaviour and properties of atoms in strong magnetic fields is a subject of increasing interest. On the o.h.s. this
is motivated by the astrophysical discovery of strong fields on white dwarfs and neutron stars [1–3] and on the o.h.s.
the competition of the diamagnetic and Coulombic interaction causes a rich variety of complex properties which are of
interest on their own. Investigations on 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 symmetry).
There are many works on the hydrogen atom (for a list of references see [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, $B_0 = \hbar c/ea_0^2 = 2.3505 \cdot 10^5$ T; atomic units 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 $\gamma$. Both early [13] and more recent works [6,17,18] 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 considered in this limit actually as 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 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 retain the separation of
the magnetic field strength domains due to decomposing 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 \[8\,9,12,14,21,23\]. The majority of them deals 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 \[22,24,27\] including calculations by Larsen \[22\] made at \(\gamma \leq 2\) for He atom and at \(\gamma \leq 5\) for H\(^-\). The latter calculations can be used for evaluations of the correlation energy in the low-field domain. HF calculations \[8\] are carried out analogously to the approach in ref. \[3\] with 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 yields therefore 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 energy 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 by Jones \textit{et al} \[11\]. 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 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 performing 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 \((\rho, \phi, z)\) with the \(z\)-axis oriented along the magnetic field. We prescribe to each electron a definite value of the magnetic quantum number \(m_\mu\). Each single-electron wave function \(\Psi_\mu\) depends on the variables \(\phi\) and \((\rho, z)\)

\[
\Psi_\mu(\rho, \phi, z) = (2\pi)^{-1/2} e^{-i m_\mu \phi} \psi_\mu(z, \rho)
\]

where \(\mu = 1, 2, 3\) is the numbering of the electrons. The resulting partial differential equations for \(\psi_\mu(z, \rho)\) and the formulæ for the Coulomb and exchange potentials have been 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 new feature which distinguishes the present calculations from those described in ref.
III. GROUND STATE ELECTRONIC CONFIGURATIONS

We start this section with a qualitative consideration of the problem of the atomic multi-electron ground states in the limit of strong magnetic fields. It is clear that the state 1s$^2$2s 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 $z$ 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 the single-electron wave functions must correspond to the lowest Landau states, i.e. $m_\mu \leq 0$ for all the electrons, and the system must be fully spin-polarized, i.e. $s_{z\mu} = -\frac{1}{2}$ (1). For the Coulomb central field the single-electron levels form quasi 1D Coulomb series with the binding energy $E_B = \frac{1}{2n_z^2}$ 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 choosen 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 [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 \[1\] 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 explicite calculations. Calculations in ref. \[11\] were carried out for configurations with the maximal single-electron principal quantum number $n \leq 2$. Under this restriction calculations for the states $1s^22s$, $1s^22p_{-1}$, $1s \downarrow 2s \downarrow 2p_{-1} \downarrow$, and $1s \downarrow 2p_0 \downarrow 2p_{-1} \downarrow$ are sufficient to determine the set of intermediate ground states. Indeed, $1s^22s$ is the zero-field ground state. $1s^22p_{-1}$ is the lowest excited state of the field free atom and (contrary to $1s^22s$) 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 $E_B$

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

in the strong field limit due to the fact that $\epsilon_B(1s) > \epsilon_B(2p_{-1}) > \epsilon_B(3d_{-2}) > \ldots \ $ in strong fields. (For $\gamma = 1000$ one can obtain binding energies from table \[1\] as $E_B(1s^22p_{-1}) = 69.1569$ and $E_B(1s^22p_{-1}3d_{-2}) = 60.0589$). The reader should note that the $1s^22p_{-1}$ 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 $n_{\mu} \leq 2$ 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, also other configurations could be considered as possible ground states for intermediate field strength. Such configurations are $1s^23s$, $1s^23p_{-1}$, $1s^23d_{-2}$, $1s2s3s$, $1s2s3p_{-1}$, $1s2s3d_{-2}$, $1s2p_{-1}3s$, 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 $1s^23s$ lies higher in energy than the $1s^22s$ configuration and that the $1s^23p_{-1}$ and $1s^23d_{-2}$ configuration possess higher energy than the $1s^22p_{-1}$ configuration. Thus, the 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 $1s2s2p_{-1}$ and the third one is significantly higher). Thus from 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 weaker bound than the $3d_{-2}$, $2p_{-1}$ and even $2p_0$ orbitals. Due to this fact also the $1s2s3s$ configuration can be excluded from becoming the ground state for any field strength. Indeed our calculations show that this state becomes higher in energy than the $1s2s2p_{-1}$ at $\gamma \approx 0.16$.

Thus, the set $1s^22p_{-1}$, $1s \downarrow 2s \downarrow 2p_{-1} \downarrow$, and $1s \downarrow 2p_0 \downarrow 2p_{-1} \downarrow$ along with weak- $1s^22s$ and strong-field $1s \downarrow 2p_{-1} \downarrow 3d_{-2} \downarrow$ ground states is comprehensive for the 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 [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 [11] the difference between [11] and our energies is 0.0239 for the 1s^22s state, 0.0205 for the 1s^22p_{-1} state, 0.0870 for the 1s2s2p_{-1} state, and 0.0458 for the 1s2p_02p_{-1} state.

Our results on the total energies are illustrated in figures 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 figures 1 and 2 that the 1s^22s configuration represents the ground state for 0 \leq \gamma < 0.17633, for 0.17633 < \gamma < 2.153 the ground state configuration is 1s^22p_{-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 [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 in compressing the electronic distribution towards the z axis. For the 1s^2p_{-1}3d_{-2} configuration for which all single-electron binding energies increase unlimited for \gamma \rightarrow \infty a shrinking process of this distribution in z direction is also visible. For the 1s^22p_{-1} configuration this effect is not distinct for the relevant field strengths. For the 1s^22s 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 \rho 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 \Sigma_s = \sum_{\mu=1}^3 s_{z \mu} = -1/2 to \Sigma_s = -3/2 for \gamma = 2.153) over the raising of the energy due to more extended charge distributions in the \rho direction.

The total binding energies of the configurations 1s^22s, 1s^22p_{-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 figure 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.

Along with the total energy of the Li atom ground state we have obtained its ionization energies \textit{E}_I dependent on \gamma. 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 [8] 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 = 2.071814. 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 figure 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}. 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 allow also obtaining ionization energies for other states presented in table I.

In addition we show in figure 6 the total quadrupole moment

\[ Q_{zz} = \langle \Psi | 3z^2 - r^2 | \Psi \rangle, \]

of different states of the atom as a function of the field strength. These dependencies illustrate the changes in the
density distribution of the electrons with increasing magnetic field strength. For weak and also to some extent for intermediate field strengths the main effect consists in compressing the wave function towards 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 towards 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 the states considered with 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 $1s^22p_{-1}$ and $1s \downarrow 2p_{-1} \downarrow 3d_{-2} \downarrow$ all these binding energies become infinite for infinite strong fields. This results in $Q_{zz} \to 0$ as $\gamma \to \infty$. For the other states presented in Figure 6 at least one of the single-electron energies remains finite as $\gamma \to \infty$ and, in result, $Q_{zz}$ has a finite limit as $\gamma \to \infty$.

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 $2.3505 \times 10^6$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 $\gamma = 0.17633$ the ground state arises from the field-free $1s^22s$ configuration. For intermediate fields ($0.17633 < \gamma < 2.1530$) the ground state is constituted by the $1s^22p_{-1}$ 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 hydrogen-like 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 $0 \leq \gamma < 2.071814$, the second one is the high-field ground state configuration for $\gamma > 2.071814$. 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 behaviour between $\gamma = 2.071814$ and $\gamma = 2.1530$. Furthermore we have studied the quadrupole moment of the atom and show how its complicated behaviour with changing field strength can be explained through the field dependence of the different HF orbitals.

Two remarks are in order. Our HF results do not include the effects of correlation. To take into account the latter would require a multiconfigurational approach which goes beyond the scope of the present paper. We, however, do not expect that the correlation energy changes our main conclusions like, for example, the transitions in the ground states configurations or the behaviour 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. For the case of hydrogen it is well-known that in the high field regime ($\gamma >> 10^2$) mass correction terms due to the finite nuclear mass become relevant i.e. are no more 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.

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 He, 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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Figure Captions

Figure 1. Total energies of the Li atom as a function of the magnetic field strength (solid lines marked by centered symbols). Dotted lines are energies of two electronic configurations of the Li$^+$ ion: (a) low-field ground state 1$s^2$; (b) high-field ground state 1$s^2$2$p_{-1}$.

Figure 2. The same as in figure 1 in the relevant regime of transitions of the ground state configurations.

Figure 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 $e$.

Figure 4. Binding energies of various states of the Li atom as a function of the magnetic field strength.

Figure 5. Li atom ground state ionization energy $E_I$ for a broad range of field strengths. 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 1$s^2$2$s$ to 1$s^2$2$p_{-1}$. The second transition corresponds to the change of the Li$^+$ ground state configuration from 1$s^2$ to 1$s^2$2$p_{-1}$. Third transition of the Li ground state configuration from 1$s^2$2$p_{-1}$ to 1$s^2$2$p_{-1}3d_{-2}$.

Figure 6. Quadrupole moment of the Li atom depending on the magnetic field strength.
### Table I. Total energies of several electronic ground and excited states of the Li atom in the regime of field strength $\gamma = 0, \ldots, 1000$

| $\gamma$ | $1s^22s$ | $1s^22p_{-1}$ | $1s2s2p_{-1}$ | $1s2p02p_{-1}$ | $1s2p_{-1}3d_{-2}$ |
|--------|----------|----------------|----------------|----------------|----------------|
|        | $E$      | $E$ [1]        | $E$            | $E$ [1]        | $E$            |
| 0.0000 | -7.43275 | -7.4327        | -7.3659        | -7.3588        | -5.2318        |
| 0.0010 | -7.43326 | -7.3669        | -5.3608        | -5.2336        | -5.0867        |
| 0.0018 | -7.43365 | -7.3669        | -5.3624        | -5.2354        | -5.0891        |
| 0.0020 | -7.43375 | -7.3670        | -5.3628        | -5.2356        | -5.0897        |
| 0.0050 | -7.43522 | -7.3700        | -5.3684        | -5.2418        | -5.0982        |
| 0.0090 | -7.43713 | -7.4371        | -5.3763        | -5.2497        | -5.1098        |
| 0.0100 | -7.43760 | -7.3748        | -5.3787        | -5.2517        | -5.1126        |
| 0.0180 | -7.44125 | -7.3821        | -5.3929        | -5.2673        | -5.1343        |
| 0.0200 | -7.44214 | -7.3839        | -5.3981        | -5.2712        | -5.1396        |
| 0.0500 | -7.45398 | -7.4084        | -5.4544        | -5.3278        | -5.2128        |
| 0.0540 | -7.45537 | -7.4114        | -5.4616        | -5.3352        | -5.2219        |
| 0.1000 | -7.46857 | -7.4417        | -5.5415        | -5.4599        | -5.3210        |
| 0.1260 | -7.47408 | -7.4565        | -5.5837        | -5.4599        | -5.3731        |
| 0.17633| -7.48162 | -7.4816        | -5.6655        | -5.5455        | -5.4756        |
| 0.1800 | -7.48204 | -7.4830        | -5.6656        | -5.5455        | -5.4756        |
| 0.2000 | -7.48400 | -7.4922        | -5.6945        | -5.5758        | -5.5151        |
| 0.5000 | -7.47741 | -7.5879        | -6.0478        | -5.9695        | -5.9705        |
| 0.5400 | -7.47351 | -7.5979        | -6.0874        | -6.0160        | -6.0241        |
| 0.9000 | -7.42504 | -7.6562        | -6.4017        | -6.3961        | -6.4606        |
| 1.0000 | -7.40879 | -7.6665        | -6.4834        | -6.4928        | -6.5708        |
| 1.2600 | -7.36226 | -7.6828        | -6.6749        | -6.7293        | -6.8412        |
| 1.8000 | -7.24603 | -7.6765        | -7.0540        | -7.1732        | -7.3472        |
| 2.0000 | -7.19621 | -7.6624        | -7.1889        | -7.3249        | -7.5200        |
| 2.07184| -7.17745 | -7.6560        | -7.2365        | -7.3779        | -7.5804        |
| 2.1530 | -7.64785 | -7.6478        | -7.6459        | -7.2945        | -7.4421        |
| 2.1600 | -7.64711 | -7.6459        | -7.2826        | -7.4421        | -7.4404        |
| 2.5000 | -7.05619 | -7.6035        | -7.5125        | -7.7182        | -7.9253        |
| 3.0000 | -6.89559 | -7.5151        | -7.8183        | -8.0837        | -8.2992        |
| 3.6000 | -6.67874 | -6.6640        | -8.1336        | -8.3721        | -8.7146        |
| 3.9600 | -7.27826 | -7.2722        | -8.3599        | -8.5739        | -8.9492        |
| 4.3200 | -7.17026 | -7.1655        | -8.5494        | -8.7745        | -9.1744        |
| 4.8600 | -7.05326 | -7.0391        | -8.7323        | -8.9632        | -9.3909        |
| 5.0000 | -6.08811 | -6.9423        | -8.8898        | -9.1255        | -9.5769        |
| 5.0400 | -6.92800 | -6.9050        | -8.9018        | -9.1456        | -9.5997        |
| 5.4000 | -5.90113 | -5.8772        | -9.0845        | -9.3213        | -9.8014        |
| 7.0000 | -5.08909 | -6.1267        | -9.7835        | -10.0386       | -10.6257       |
| 10.00  | -3.35777 | -4.6177        | -10.9105       | -11.1788       | -11.9390       |
| 20.00  | 3.49120  | 1.7056         | -13.6942       | -13.9658       | -15.1620       |
| 50.00  | 27.6916  | 24.9794        | -18.8012       | -19.0436       | -21.0505       |
| 100.00 | 71.807   | 68.1735        | -23.987        | -24.1946       | -27.0192       |
| 200.00 | 164.371  | 159.5749       | -30.559        | -30.7327       | -34.5850       |
| 500.00 | 451.69   | 444.9033       | -41.821        | -41.959        | -47.5583       |
|     |      |      |      |      |      |
|-----|------|------|------|------|------|
| 1000 | 939.54 | 930.84308 | -52.65 | -52.771 | -60.0589 |
TABLE II. Energies 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 $\gamma = 0, \ldots, 1000$.

| $\gamma$  | $1s^2$     | $1s2p_{-1}$ | $E_I$(Li) |
|----------|------------|-------------|-----------|
| 0.0000   | -7.23642   | -5.02469    | 0.19633   |
| 0.0010   | -7.23642   | -5.02619    | 0.19684   |
| 0.0020   | -7.23642   | -5.02769    | 0.19733   |
| 0.0050   | -7.23641   | -5.03218    | 0.19881   |
| 0.0100   | -7.23641   | -5.03963    | 0.20119   |
| 0.0200   | -7.23639   | -5.05442    | 0.20575   |
| 0.0500   | -7.23623   | -5.09797    | 0.21775   |
| 0.1000   | -7.23567   | -5.16789    | 0.23290   |
| 0.17633  | -7.23411   | -5.26874    | 0.24751   |
| 0.2000   | -7.23345   | -5.29873    | 0.25875   |
| 0.5000   | -7.21798   | -5.64006    | 0.36992   |
| 1.0000   | -7.16401   | -6.11462    | 0.50252   |
| 2.0000   | -6.96300   | -6.89408    | 0.69946   |
| 2.071814 | -6.94440   | -6.94440    | 0.71160   |
| 2.1530   | -6.92278   | -7.00057    | 0.64729   |
| 2.5000   | -6.82347   | -7.23258    | 0.69275   |
| 3.0000   | -6.66237   | -7.54672    | 0.75248   |
| 5.0000   | -5.85051   | -8.62943    | 0.94751   |
| 7.0000   | -4.84725   | -9.52492    | 1.10086   |
| 10.      | -3.11092   | -10.65131   | 1.28771   |
| 20.      | 3.74896    | -13.42974   | 1.73286   |
| 50.      | 27.96465   | -18.52548   | 2.5250    |
| 100.     | 72.09337   | -23.69994   | 3.3193    |
| 200.     | 164.66867  | -30.26077   | 4.3242    |
| 500.     | 452.0032   | -41.50393   | 6.0544    |
| 1000.    | 939.87976  | -52.3230    | 7.7359    |
BINDING ENERGY

$1s^2 2s$

$1s^2 2p_{-1}$

$1s2s2p_{-1}$

$1s2p_{-1}3d_{-2}$

$1s2p_{0}2p_{-1}$

$log_{10} \gamma$
GROUND STATE IONIZATION ENERGY

\[ \log_{10} \gamma \]
