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# Density-functional calculations in a two-dimensional finite-element basis for atoms in very strong magnetic fields: Energy values

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Results of density-functional calculations for atoms in very strong magnetic fields using a two-dimensional finite-element basis set are reported for ground-state energies of helium, carbon, and neon, and for some excited states of helium. We give results obtained by using three different local-density functionals. A comparison with multi-Landau-channel Hartree-Fock calculations shows reasonable agreement for helium.

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## I. INTRODUCTION

The properties of atoms in very strong magnetic fields have been the subject of many research efforts during the last three decades. Noteworthy are the investigations on Wannier excitons by Fritsche and co-workers [1,2], the paper by Canuto and Ventura [3], and the many publications in this field from the group of Ruder and Wunner in Erlangen und Tübingen; see Refs. [4–7] and references therein. This is, on the one hand, due to the discovery of very strongly magnetized objects in the universe, in particular, white dwarfs [8] and neutron stars [9]. On the other hand, the topic of the dynamics of quantum systems under the influence of the competing symmetries of Coulomb and Lorentz forces has by itself been a strong motivation. In addition, there have also been developments in solid-state physics, which gave additional impetus for this research field.

For hydrogen and hydrogenlike systems, the calculations have now reached a very complete level [10]. However, for many-electron atoms beyond helium, nearly all calculations have so far been done in the adiabatic approximation, which assumes that the one-particle wave functions are in cylindrical coordinates $\rho, z, \phi$ given by a product of a function of $z$ and the eigenfunctions of the two-dimensional harmonic oscillator or Landau functions in $\rho$ and $\phi$. Two examples for this approach are the Hartree-Fock calculations by Miller [11] and the heuristic density-functional calculations by Jones [12]. Thus, one assumes that the electron only occupies the lowest Landau level for a given value of the magnetic quantum number $m$. There have been some efforts to improve on this by adding more Landau channels [13].

The use of density-functional-theory techniques for many-electron atoms is an attractive option, since it does not involve the calculation of computationally intensive exchange integrals.

Already more than 10 years ago, Vignale and Rasolt have developed [14–17] the theoretical framework of a current density-functional theory applicable to our current problem. In their formalism, the exchange-correlation functional also depends on the paramagnetic current density. However, the exchange-correlation energy is a portion of the total electron-electron interaction energy, which in a nonrelativistic description, and if one neglects the current-current, current-spin, and spin-spin interactions between the electrons, all of which are many orders of magnitude smaller than the influence of the external magnetic field, does not involve the current density. There is of course a rather strong indirect dependence in the sense that the magnetic field changes the densities from the field-free case. Thus we can drop the direct current dependence from the functionals in the one-particle equations obtained by Vignale and co-workers and simply use the density-dependent functionals as they have been used in the field-free case.

In this paper, we will report on the results of density-functional calculations in cylindrical coordinates employing a two-dimensional finite element basis in $\rho$ and $z$. This allows, in principle, for a smooth connection to the low-field domain, since the details of the grid can be adopted to the strength of the magnetic field, and there are, apart from the cusp condition at the origin, no difficulties in obtaining low-field solutions in this basis set. Even this problem is not of major consequence for the accuracy of the wave functions, if the grid is suitably concentrated at the origin. However, in this paper, we will treat only the case of very strong magnetic fields and there only consider the spin-polarized case, where all spins are antiparallel to the magnetic field, which is energetically favored.

The paper is organized as follows: in Sec. II, we show the Hamiltonian. In Sec. III, we describe our ansatz. In Sec. IV, we discuss the numerical method used, while in Sec. V, some results of our calculations are presented. Finally, in Sec. VI, we present our conclusions.

## II. THE HAMILTONIAN

We consider an atom consisting of $n_e$ electrons and a nucleus of charge $Ze$ in a homogeneous magnetic field $B$ along the $z$ axis. Using $Z$-scaled atomic units, i.e., as energy unit $E_Z = Z^2$ Rydberg and as length unit $a_{\mathrm{Bohr}}/Z$, neglecting the finite mass of the nucleus, and choosing the following cylindrically symmetric gauge, i.e., the vector potential as

$$\boldsymbol{A} = \beta_Z \boldsymbol{e}_z \times \boldsymbol{r}, \tag{1}$$

the Hamiltonian reads in cylindrical coordinates $(\rho_i, z_i, \phi_i)$

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$$H=\sum_{i=1}^{n_e}\left[-\frac{1}{\rho_i}\frac{\partial}{\partial\rho_i}\rho_i\frac{\partial}{\partial\rho_i}+\frac{l_{z_i}^2}{\rho_i^2}-\frac{\partial^2}{\partial z_i^2}-\frac{2}{\sqrt{\rho_i^2+z_i^2}}\right.$$
$$\left.+2\beta_Z[l_{z_i}+2s_{z_i}]+\beta_Z^2\rho_i^2\right]+\frac{2}{Z}\sum_{i>j}^{n_e}$$
$$\times\frac{1}{\sqrt{\rho_i^2+\rho_j^2-2\cos(\phi_i-\phi_j)\rho_i\rho_j+(z_i-z_j)^2}},\qquad(2)$$

with $\beta_Z=B/(Z^2\times4.7010\times10^5\ \text{T})$ and the $z$ components $l_{z_i}$, $s_{z_i}$ of the angular-momentum operator and spin for the $i$th electron in units of $\hbar$. Neglecting the finite mass of the nucleus has two effects: first, the well-known mass-polarization effect that is present irrespective of the strength of the magnetic field and the corrections due to the motion of the charged nucleus in the magnetic field, which will grow with $\beta_Z$. Thus the energies obtained for very large $\beta_Z$ values of the order 1000 have to be considered as rather approximative values.

For very strong magnetic fields, i.e., $\beta_Z\gtrsim1$, the spin-flip energy of $4\beta_Z E_Z$ per electron means that all electrons will be in a spin-down state for the ground state and many low-lying states. Thus the space part of the wave function will be totally antisymmetric. For the remainder of this paper, we only consider states of this kind and suppress the spin degrees of freedom.

## III. THE ANSATZ FOR THE WAVE FUNCTION

We will describe the wave function by a single Slater determinant $\Psi$ constructed from suitably chosen one-electron wave functions $\Phi_i$, i.e.,

$$\Psi(\boldsymbol{r}_1,\boldsymbol{r}_2,\ldots,\boldsymbol{r}_{n_e})$$
$$=\frac{1}{\sqrt{n_e!}}\sum_P(-1)^P P\Phi_1(\boldsymbol{r}_1)\Phi_2(\boldsymbol{r}_2)\cdots\Phi_{n_e}(\boldsymbol{r}_{n_e}),\qquad(3)$$

where $P$ is the permutation operator. Calculating the expectation value $\langle H\rangle$ for this ansatz, we obtain

$$\langle H\rangle=\sum_i\langle\Phi_i|-\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{l_z^2}{\rho^2}-\frac{\partial^2}{\partial z^2}-\frac{2}{\sqrt{\rho^2+z^2}}$$
$$+2\beta_Z[l_z+2s_z]+\beta_Z^2\rho^2|\Phi_i\rangle+\frac{2}{Z}\frac{1}{2}\sum_{i,j}\int d\boldsymbol{r}$$
$$\times\int d\boldsymbol{r}'\,\Phi_i^*(\boldsymbol{r})\Phi_j^*(\boldsymbol{r}')\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}\Phi_i(\boldsymbol{r})\Phi_j(\boldsymbol{r}')-\frac{2}{Z}\frac{1}{2}$$
$$\times\sum_{i,j}\int d\boldsymbol{r}\int d\boldsymbol{r}'\,\Phi_j^*(\boldsymbol{r})\Phi_i^*(\boldsymbol{r}')\frac{1}{|\boldsymbol{r}-\boldsymbol{r}'|}\Phi_i(\boldsymbol{r})\Phi_j(\boldsymbol{r}').$$
$$(4)$$

Looking for an extremum of the energy under the orthogonality conditions

$$\langle\Phi_i|\Phi_j\rangle=\delta_{ij},\qquad(5)$$

requiring $n_e^2$ Lagrange multipliers $\epsilon_{ij}$ we obtain the well known Hartree-Fock equations which in the units defined above read

$$\left\{-\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{l_z^2}{\rho^2}-\frac{\partial^2}{\partial z^2}-\frac{2}{\sqrt{\rho^2+z^2}}+2\beta_Z[l_z+2s_z]\right.$$
$$\left.+\beta_Z^2\rho^2+\frac{2}{Z}\int\frac{n(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}d\boldsymbol{r}'\right\}\Phi_i(\boldsymbol{r})$$
$$-\frac{2}{Z}\int\sum_j\frac{\phi_j(\boldsymbol{r})\phi_j^*(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}\Phi_i(\boldsymbol{r}')d\boldsymbol{r}'=\sum_j\epsilon_{ij}\phi_j(\boldsymbol{r}),$$
$$(6)$$

with the density

$$n(\boldsymbol{r})=\sum_i\Phi_i^*(\boldsymbol{r})\Phi_i(\boldsymbol{r}).\qquad(7)$$

It is now customary to specialize to the case $\epsilon_{ij}=\delta_{ij}\epsilon_i$, which can always be achieved by applying a rotation to the vector of wave functions $(\Phi_i)$.

The nonlocal exchange terms in the above equations make, however, the application of the Hartree-Fock method very demanding in terms of computational power, since a large number of matrix elements of the type $\langle ij|1/r_{12}|kl\rangle$ have to be evaluated. Therefore, the density-functional approach, where the exchange term in Eq. (4) is approximated by a functional of the one-particle density $n$, is more convenient and should, for the purposes of this calculation, still be accurate enough. In addition, the density-functional approach allows for the inclusion of correlation effects at least in principle. We have, however, to keep in mind that the density-functional approach is normally restricted to ground states. In this work, we use it for low-lying excited states as well, which can be justified along the lines of a generalized Kohn-Sham approach [19–21], where it is shown, that state-dependent local functionals exist that lead to Slater determinants that have the correct one-particle density. Thus, we admittedly use the density-functional approach in a heuristic manner, since the exact functionals are not known, but this is the case with most of the current application of the density-functional theory.

In the following we restrict ourselves to the so-called local-density approximation, where the exchange and correlation functional is expressed as

$$E_{xc}[n]=\int n(\boldsymbol{r})e_{xc}(n(\boldsymbol{r}))d\boldsymbol{r},\qquad(8)$$

leading to a local potential

$$v_{xc}(\boldsymbol{r})=n(\boldsymbol{r})\frac{\partial e_{xc}}{\partial n}+e_{xc}(n(\boldsymbol{r})). \tag{9}$$

Thus, we use the following self-consistent one-particle Hamiltonian for an electron with spin $-1/2$ and magnetic quantum number $m\leqslant 0$,

$$H_{\mathrm{eff}\,m}=-\frac{1}{\rho}\frac{\partial}{\partial\rho}\rho\frac{\partial}{\partial\rho}+\frac{m^2}{\rho^2}-\frac{\partial^2}{\partial z^2}-\frac{2}{\sqrt{\rho^2+z^2}}-2\beta_Z[|m|+1]+\beta_Z^2\rho^2+\frac{2}{Z}\left\langle\int\frac{n(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}d\boldsymbol{r}'\right\rangle_\phi+\langle v_{xc}(\boldsymbol{r})\rangle_\phi, \tag{10}$$

where $\langle\cdots\rangle_\phi$ stands for the average over the azimuthal angle, with associated eigenvalues $\epsilon_i$. Since the potentials in question are cylindrically symmetric, this average is equivalent to taking the potentials at $\phi=0$. Evaluating the expectation value of $\langle H\rangle$ for our density-functional approach, we obtain

$$E=\sum_i\epsilon_i-\frac{2}{Z}\frac{1}{2}\int\frac{n(\boldsymbol{r}')n(\boldsymbol{r})}{|\boldsymbol{r}-\boldsymbol{r}'|}d\boldsymbol{r}\,d\boldsymbol{r}'+\int n(\boldsymbol{r})e_{xc}(n(\boldsymbol{r}))d\boldsymbol{r}-\int n(\boldsymbol{r})v_{xc}(n(\boldsymbol{r}))d\boldsymbol{r}. \tag{11}$$

The low-lying eigenstates of the effective Hamiltonian (10) can be classified in analogy to those of hydrogen in a strong magnetic field as detailed in Chap. 4 of Ref. [10]. For purpose of this classification, it is convenient to consider the adiabatic approximation, where the $(\rho,z)$-dependent portion of the wave function is assumed to have the form

$$\Psi_{lm\nu}=\frac{1}{N_{lm}}(\rho\sqrt{\beta_Z})^{|m|}L_{l+|m|}^{|m|}\exp\left(-\frac{1}{2}\beta_Z^2\rho^2\right)F_\nu^{(lm)}(z), \tag{12}$$

with $l$ instead of the customary $n$, indicating the Landau levels, the Laguerre polynomials $L_\beta^\alpha$, a normalization constant $N_{lm}$ that is not of further interest here, and where $F_\nu^{(lm)}$ is a solution of the one-dimensional Schrödinger equation

$$\left[-\frac{\partial^2}{\partial z^2}+V_{\mathrm{eff}}^{(lm)}(z)\right]F_\nu^{(lm)}(z)=\epsilon_\nu^{(lm)}F_\nu^{(lm)}(z). \tag{13}$$

The $l$ and $m$-dependent effective potential $V_{\mathrm{eff}}^{(lm)}$ is defined by

$$V_{\mathrm{eff}}^{(lm)}(z)=\int_0^\infty R_{lm}(\rho)^2\left[-\frac{2}{\sqrt{\rho^2+z^2}}+\left\langle\frac{2}{Z}\int\frac{n(\boldsymbol{r}')}{|\boldsymbol{r}-\boldsymbol{r}'|}d\boldsymbol{r}'\right\rangle_\phi+\langle v_{xc}(\boldsymbol{r})\rangle_\phi\right]\rho\,d\rho, \tag{14}$$

where $R_{lm}(\rho)$ denotes the $\rho$-dependent part on the right-hand side of Eq. (12) and $\nu$ denotes the number of nodes of $F_\nu^{(lm)}$. Thus the one-particle energies of these wave functions are obtained as

$$e_\nu^{(lm)}=\beta_Z(2l+|m|+m)+\epsilon_\nu^{(lm)}. \tag{15}$$

Since we are considering the case of $\beta_Z\gtrsim 1$, we will further restrict ourselves to $l=0$, since states with $l>0$, because of the term $2\beta_Z l$, do not belong to the low lying part of the spectrum.

Thus, the eigenstates can be labeled by $(m,\nu)$ with the magnetic quantum number $m\leqslant 0$ and the node number $\nu\geqslant 0$, where even (odd) $\nu$ refers to even (odd) $z$ parity. The reason that only $m\leqslant 0$ will be considered is that positive values of $m$ incur a penalty of $4\beta_Z mE_Z$ relative to negative $m$ values and thus are not considered for $\beta_Z\gtrsim 1$. The spectrum of this effective Hamiltonian can also be expected to be qualitatively similar to that of hydrogen in a magnetic field, insofar as the lowest states start with a number $n_s$ of strongly bound states $(m,0)$, i.e., states whose binding energies grow without bound if $\beta_Z$ is increased in contrast to the hydrogenlike states $(m,\nu>0)$ whose energies approach limiting values for $\beta_Z$ to $\infty$. $n_s$ also grows with $\beta_Z$.

This means that the ground state for our system will, for sufficiently large values of $\beta_Z$, be obtained as a Slater determinant of strongly bound states with increasing values of $|m|$ and that there will be, for each value of $Z$ and $n_e$, a critical magnetic field $\beta_Z$ below which the ground state contains at least one electron that is *not* strongly bound, i.e., for which $\nu>0$. In this work, we will, however, restrict ourselves to values of $\beta_Z$, such that the ground state consists of only strongly bound states. In this paper, we shall denote the atomic eigenstates by the occupied single-electron states. For example, the ground state of carbon will be labeled by $|(0,0)(-1,0)(-2,0)(-3,0)(-4,0)(-5,0)\rangle$.

The low-lying excited states can be obtained by either exciting one electron to higher values of $|m|$ or by exciting it to a hydrogenlike state, i.e., to $\nu>0$. Those of the first type will be quite close in energy to the ground-state energy, since changing $m$ results in a small change of the one-particle energies, especially for $m\gg 1$, while those of the second type will be more strongly excited, since the binding energy of a hydrogenlike state is small compared to that of a strongly bound state.

In the last 30 years, many expressions for the exchange and correlation functional have been suggested [18]. In this work, we will make use of three of them, namely the spin-polarized exchange functional for the free electron gas dating back to Dirac [13]

$$e_{\mathrm{Dirac}}(n(\boldsymbol{r}))=-\frac{1}{Z}\frac{3}{2}\left(\frac{6}{\pi}\right)^{1/3}[n(\boldsymbol{r})]^{1/3}, \tag{16}$$

the expression due to Fritsche [19],

$$e_{\mathrm{Fritsche}}(n(\boldsymbol{r}))=-\frac{2}{Z}[n(\boldsymbol{r})]^{1/3}, \tag{17}$$

derived by assuming a Gaussian correlation factor, which differs from the above only by a factor, and the heuristic functional due to Jones [12], which also includes a correlation term,

TABLE I. Energy values obtained for the ground state $|(0,0)(-1,0)\rangle$ of helium calculated by using the functionals due to Dirac, Fritsche, and Jones. For comparison, the extrapolated results of a multi-Landau-channel Hartree-Fock calculation [6] are also shown.

| $\beta_Z$ | $E_{\mathrm{Dirac}}$ | $E_{\mathrm{Fritsche}}$ | $E_{\mathrm{Jones}}$ | $E_{\mathrm{MCHF}}$ |
|---|---|---|---|---|
| 1 | −2.6253 | −2.6783 | −2.7973 | −2.8008 |
| 2 | −3.3521 | −3.4205 | −3.5560 | −3.5150 |
| 5 | −4.6693 | −4.7666 | −4.9300 | −4.8051 |
| 10 | −6.0044 | −6.1323 | −6.3115 | −6.0991 |
| 20 | −7.7047 | −7.8733 | −8.0571 | −7.7228 |
| 50 | −10.6517 | −10.8948 | −11.0528 | −10.4714 |
| 100 | −13.5523 | −13.8571 | −13.9710 | −13.085 |
| 200 | −17.1200 | −17.5425 | −17.5253 | −16.229 |
| 500 | −23.2204 | −23.8283 | −23.5341 | −21.312 |
| 1000 | −29.2970 | −29.9930 | −29.3533 | −25.94 |

$$e_{\mathrm{Jones}}(n(\boldsymbol{r}))=\frac{1}{Z}\Bigg[\frac{2\pi n\ln n}{\beta_Z}-3\pi n\frac{\ln 2\beta_Z}{\beta}+13.7\frac{n}{\beta_Z}-37.8\,\frac{n^2}{\sqrt{8}\beta_Z^{2.5}}-\sqrt{8\beta_Z}[0.0096\ln\,n-0.0144\ln 2\beta_Z+0.122]\Bigg]. \tag{18}$$

In all three expressions above $n(\boldsymbol{r})$ denotes the spin-down density, which is identical to the total density for the case we are considering.

From the above functionals, the potentials are found as

$$v_{\mathrm{Dirac}}(\boldsymbol{r})=-\frac{2}{Z}\left(\frac{6}{\pi}\right)^{1/3}[n(\boldsymbol{r})]^{1/3}, \tag{19}$$

$$v_{\mathrm{Fritsche}}(\boldsymbol{r})=-\frac{2}{Z}\frac{4}{3}[n(\boldsymbol{r})]^{1/3}, \tag{20}$$

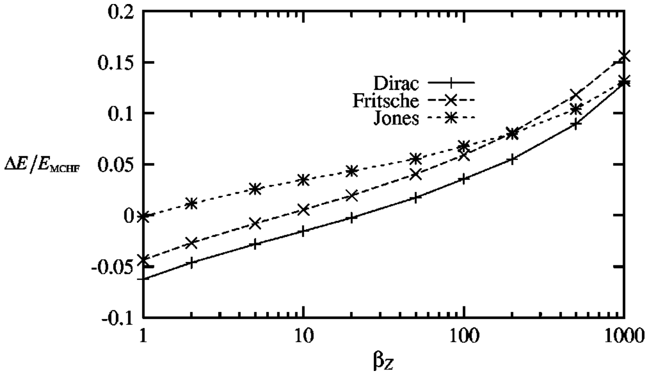

FIG. 1. Relative difference between the ground-state energies obtained using the functionals due to Dirac, Fritsche, and Jones and the multichannel Hartree-Fock energies [6]. Positive values correspond to overbinding.

TABLE II. Energy values obtained for the ground states of helium, carbon, and neon, calculated with different numerical methods using the functional due to Jones at $\beta_Z$ values corresponding to $2\times10^8$ T and $5\times10^8$ T. The results denoted by $E_{\mathrm{Jones}}$ are taken from Ref. [12], those denoted by $E_{\mathrm{Relovsky}}$ are from Ref. [22], and our results are shown in the rightmost column.

| $Z$ | $\beta_Z$ | $B(10^8$ T) | $E_{\mathrm{Jones}}$ | $E_{\mathrm{Relovsky}}$ | $E$ |
|---|---|---|---|---|---|
| 2 | 265.9 | 5 | −19.11 | −19.15 | −19.21 |
| 6 | 29.54 | 5 | −16.39 | −16.35 | −16.41 |
| 10 | 4.254 | 2 | −10.41 | −10.36 | −10.57 |
| 10 | 10.64 | 5 | −14.88 | −14.84 | −15.02 |

$$v_{\mathrm{Jones}}(\boldsymbol{r})=\frac{1}{Z}\Bigg[\frac{2\pi(n+2n\ln n)}{\beta_Z}-6\pi n\frac{\ln 2\beta_Z}{\beta}+27.4\,\frac{n}{\beta_Z}-113.4\,\frac{n^2}{\sqrt{8}\beta_Z^{2.5}}-\sqrt{8\beta_Z}[0.0096(1+\ln n)-0.0144\ln 2\beta_Z+0.122]\Bigg]. \tag{21}$$

## IV. NUMERICAL METHOD

### A. Expansion of the one-electron wave function

The one-electron wave functions for a particular combination of $m$ and $\nu$ are taken as

$$\Phi_{m\nu}=\exp(im\phi)\psi_{m\nu}(\rho,z), \tag{22}$$

where the reduced wave functions $\psi_{m\nu}$ are expanded in terms of localized finite-element functions, which are spliced together from Lagrange interpolation polynomials of order $N$ on grids in both $\rho$ and $z$. Thus,

$$\psi_{m\nu}=\sum_i c_i^{(m\nu)}F_i(\rho,z), \tag{23}$$

where the $F_i$ will of course depend on the details of the discretization, as well as the boundary conditions and the coefficients $c_i$ are the values of the reduced wave functions at the chosen grid points in the $\rho$-$z$ plane. Since the $z$ parity is a good quantum number of the system, we restrict ourselves to $z\geqslant0$. The boundary conditions at $\rho=0$ and $z=0$, are then given as follows:

$$\Psi(0,z)=0\quad\text{for}\ \ m>0, \tag{24}$$

$$\Psi(0,z)\quad\text{open for}\ \ m=0, \tag{25}$$

$$\Psi(\rho,0)=0\quad\text{for}\ \ \nu=2\lambda+1, \tag{26}$$

$$\Psi(\rho,0)\quad\text{open for}\ \ \nu=2\lambda. \tag{27}$$

TABLE III. Ground-state energies of carbon and neon in very strong magnetic fields calculated using the functional due to Fritsche.

| $\beta_Z$ | $E_{\mathrm{C}}$ | $E_{\mathrm{Ne}}$ |
|---|---|---|
| 1 | −4.5712 | −5.9184 |
| 2 | −5.9496 | −7.7814 |
| 5 | −8.4396 | −11.1422 |
| 10 | −10.9659 | −14.5564 |
| 20 | −14.1887 | −18.9215 |
| 50 | −19.7819 | −26.5179 |
| 100 | −25.2554 | −33.9694 |
| 200 | −32.0330 | −43.2098 |
| 500 | −43.4474 | −58.7362 |
| 1000 | −54.2638 | −73.5062 |

### B. The discretization

The grids in $\rho$ and $z$ are generated from a choice of $\rho_{\max}$ and $z_{\max}$ via

$$R_i=\left(\frac{i}{n_\rho}\right)^2\rho_{\max}, \tag{28}$$

$$Z_i=\left(\frac{i}{n_z}\right)^2 z_{\max}. \tag{29}$$

In each rectangular element of the form $[R_i,R_{i+1}]\times[Z_i,Z_{i+1}]$, the interpolation nodes will, however, be distributed uniformly, because the Lagrange interpolation polynomials have equidistant nodes.

The cutoff in $\rho$ is chosen as

$$\rho_{\max}=\frac{\sqrt{m_{\max}}+3}{\sqrt{\beta_Z}}, \tag{30}$$

where $m_{\max}$ is the largest value of $|m|$ needed. This choice can be motivated from the minimum of the effective potential at $z=0$, which is, excluding the coulomb terms, given by $(m^2/\rho^2)+\beta_Z^2\rho^2$, yielding $\rho_{\min}=\sqrt{m/\beta_Z}$. Although this argument neglects the Coulomb potential it turns out, that the densities obtained will have their maxima at this $\rho_{\min}$ with very high precision, since except for the immediate vicinity of the nucleus, the Coulomb force is, especially for $\beta_Z>1$, weaker than the Lorentz force, and thus can only result in a small shift.

TABLE IV. Energies of the state $|(0,0)(-1,1)\rangle$ of helium in very strong magnetic fields calculated using the functionals due to Dirac, Fritsche, and Jones with the MCHF results for comparison in the rightmost column.

| $\beta_Z$ | $E_{\mathrm{Dirac}}$ | $E_{\mathrm{Fritsche}}$ | $E_{\mathrm{Jones}}$ | $E_{\mathrm{MCHF}}$ |
|---|---|---|---|---|
| 1 | −2.1735 | −2.2156 | −2.2788 | −2.2474 |
| 2 | −2.7171 | −2.7698 | −2.8261 | −2.7750 |
| 5 | −3.6949 | −3.7675 | −3.8175 | −3.7218 |
| 10 | −4.6790 | −4.7724 | −4.8101 | −4.6658 |
| 20 | −5.9247 | −6.0455 | −6.0605 | −5.8446 |
| 50 | −8.0687 | −8.2396 | −8.1989 | −7.8301 |
| 100 | −10.1611 | −10.3763 | −10.2706 | −9.708 |
| 200 | −12.7248 | −13.0166 | −12.7899 | −11.959 |
| 500 | −17.0343 | −17.4506 | −16.9831 | −15.577 |
| 1000 | −21.1146 | −21.6589 | −20.9092 | −18.86 |

TABLE V. Energies of the state $|(0,0)(-2,0)\rangle$ of helium in very strong magnetic fields calculated using the functionals due to Dirac, Fritsche, and Jones with the MCHF results for comparison in the rightmost column.

| $\beta_Z$ | $E_{\mathrm{Dirac}}$ | $E_{\mathrm{Fritsche}}$ | $E_{\mathrm{Jones}}$ | $E_{\mathrm{MCHF}}$ |
|---|---|---|---|---|
| 1 | −2.4518 | −2.4987 | −2.5857 | −2.5580 |
| 2 | −3.1260 | −3.1864 | −3.2790 | −3.2169 |
| 5 | −4.3511 | −4.4374 | −4.5394 | −4.4100 |
| 10 | −5.5948 | −5.7085 | −5.8090 | −5.6100 |
| 20 | −7.1799 | −7.3301 | −7.4152 | −7.1198 |
| 50 | −9.9288 | −10.1457 | −10.1753 | −9.6840 |
| 100 | −12.6342 | −12.9066 | −12.8665 | −12.130 |
| 200 | −15.9602 | −16.3378 | −16.1458 | −15.082 |
| 500 | −21.5955 | −22.1390 | −21.6445 | −19.871 |
| 1000 | −26.9775 | −27.6923 | −26.8399 | −24.25 |

The choice of $z_{\max}$ depends very much on whether hydrogenlike, i.e., loosely bound states with $\nu>0$ are required. If they are not needed, i.e., if only nodeless states are required, the choice

$$z_{\max}\sim\frac{7}{\sqrt{|E_{-m_{\max}0}|}} \tag{31}$$

will be appropriate since the electron with the highest $|m|$ will be the most loosely bound and the decay of the wave function in $z$ direction is governed by its binding energy. This choice means that the exact one-particle densities will at this value decay to about $10^{-6}$ of their value at $z=0$. Since the binding energies needed above scale approximately with

TABLE VI. Energies of the state $|(0,0)(-2,1)\rangle$ of helium in very strong magnetic fields calculated using the functionals due to Dirac, Fritsche, and Jones with the MCHF results for comparison in the rightmost column.

| $\beta_Z$ | $E_{\mathrm{Dirac}}$ | $E_{\mathrm{Fritsche}}$ | $E_{\mathrm{Jones}}$ | $E_{\mathrm{MCHF}}$ |
|---|---|---|---|---|
| 1 | −2.1507 | −2.1910 | −2.2484 | −2.2288 |
| 2 | −2.6927 | −2.7432 | −2.7940 | −2.7592 |
| 5 | −3.6673 | −3.7371 | −3.7838 | −3.7101 |
| 10 | −4.6473 | −4.7372 | −4.7744 | −4.6570 |
| 20 | −5.8867 | −6.0032 | −6.0210 | −5.8384 |
| 50 | −8.0173 | −8.1824 | −8.1497 | −7.8263 |
| 100 | −10.0945 | −10.3023 | −10.2090 | −9.706 |
| 200 | −12.6372 | −12.9194 | −12.7099 | −11.957 |
| 500 | −16.9070 | −17.3100 | −16.8658 | −15.576 |
| 1000 | −20.9458 | −21.4728 | −20.7499 | −18.86 |

TABLE VII. Energies of the state $|(0,0)(-3,0)\rangle$ of helium in very strong magnetic fields calculated using the functionals due to Dirac, Fritsche, and Jones with the MCHF results for comparison in the rightmost column.

| $\beta_Z$ | $E_{\rm Dirac}$ | $E_{\rm Fritsche}$ | $E_{\rm Jones}$ | $E_{\rm MCHF}$ |
|---|---|---|---|---|
| 1 | $-2.3696$ | $-2.4133$ | $-2.4833$ | $-2.4634$ |
| 2 | $-3.0151$ | $-3.0712$ | $-3.1405$ | $-3.0995$ |
| 5 | $-4.1895$ | $-4.2695$ | $-4.3395$ | $-4.2518$ |
| 10 | $-5.3821$ | $-5.4874$ | $-5.5487$ | $-5.4116$ |
| 20 | $-6.9020$ | $-7.0410$ | $-7.0792$ | $-6.8719$ |
| 50 | $-9.5368$ | $-9.7377$ | $-9.7105$ | $-9.3542$ |
| 100 | $-12.1284$ | $-12.3804$ | $-12.2767$ | $-11.724$ |
| 200 | $-15.3120$ | $-15.6621$ | $-15.4035$ | $-14.587$ |
| 500 | $-20.6981$ | $-21.2019$ | $-20.6431$ | $-19.237$ |
| 1000 | $-25.8274$ | $-26.4900$ | $-25.5832$ | $-23.49$ |

$\sqrt{\beta_Z}$, the optimal value of $z_{\rm max}$ only shows a weak dependence on $\beta_Z$. However, if loosely bound states are needed, the $z$ range will have to be increased considerably, which makes the computational effort required larger, since $n_z$ will have to be larger as well.

If one of the electrons is excited to a hydrogenlike state with $\nu > 0$, its binding energy can in our units, using an oversimplified, but sufficient picture, where all other electrons and the nucleus are assumed to act as central charge of $(1+Z-n_e)e$, be estimated as

$$|E_{m\nu}| = \frac{(1+q)^2}{Z^2\nu^2}, \tag{32}$$

with the total charge of the system $q = Z - n_e$.

Estimating the effective potential in the $Z$-scaled units as

$$v_{\rm eff}(z) = -2\frac{1+q}{Z}\frac{1}{|z|}, \tag{33}$$

we easily obtain the following rough estimate for the cutoff in $z$,

$$z_{\rm max} \gtrsim 2\frac{Z}{1+q}\nu^2. \tag{34}$$

TABLE VIII. Energies of the state $|(0,0)(-3,1)\rangle$ of helium in very strong magnetic fields calculated using the functionals due to Dirac, Fritsche, and Jones with the MCHF results for comparison in the rightmost column.

| $\beta_Z$ | $E_{\rm Dirac}$ | $E_{\rm Fritsche}$ | $E_{\rm Jones}$ | $E_{\rm MCHF}$ |
|---|---|---|---|---|
| 1 | $-2.1370$ | $-2.1764$ | $-2.2321$ | $-2.2182$ |
| 2 | $-2.6780$ | $-2.7273$ | $-2.7769$ | $-2.7501$ |
| 5 | $-3.6507$ | $-3.7188$ | $-3.7657$ | $-3.7034$ |
| 10 | $4.6283$ | $-4.7162$ | $-4.7550$ | $-4.6522$ |
| 20 | $-5.8639$ | $-5.9779$ | $-5.9990$ | $-5.8353$ |
| 50 | $-7.9864$ | $-8.1482$ | $-8.1213$ | $-7.8251$ |
| 100 | $-10.0539$ | $-10.2575$ | $-10.1720$ | $-9.706$ |
| 200 | $-12.5826$ | $-12.8593$ | $-12.6595$ | $-11.958$ |
| 500 | $-16.8235$ | $-17.2188$ | $-16.7861$ | $-15.577$ |
| 1000 | $-20.8282$ | $-21.3452$ | $-20.6337$ | $-18.86$ |

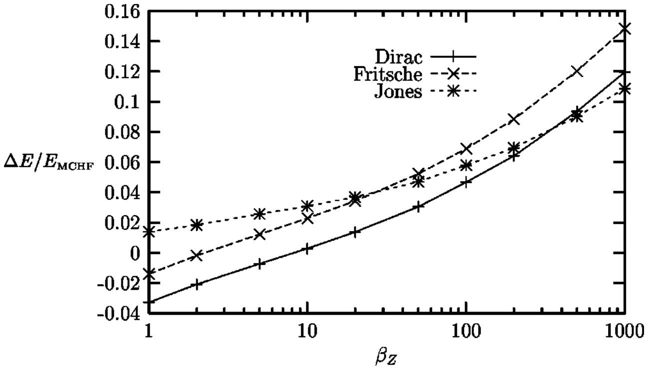

FIG. 2. As in Fig. 1, but for the $|(0,0)(-1,1)\rangle$ state of helium.

The evaluation of matrix elements with respect to the finite-element basis functions is accomplished by Gauss-Legendre integration over the elements defined above, except for the element at the origin, where the rectangular element is transformed to a curvilinear domain in spherical coordinates $r$ and $\theta$, which is then treated by two separate Gauss-Legendre integrations. This is done to ensure the accurate integration of terms containing the Coulomb potential $2/\sqrt{\rho^2+z^2}$. The global integrals required to obtain the total energy (11) are evaluated using the same grid. In the calculations to be reported, we used a global grid of $12\times 12$ elements in $\rho$ and $z$, $12\times 12$ Gauss-Legendre integration points per element and the interpolation polynomials were of order $N=4$. The Coulomb potential due to the axially symmetric charge distribution $n(\boldsymbol{r})$ was evaluated by the use of Fourier-Bessel transforms, as detailed in Appendix B of Ref. [12].

### C. Self-consistent procedure

The equations resulting from our density-functional ansatz have to be solved by iteratively finding the $n_e$ selected eigenstates of Eq. (10) until self-consistency is reached, which we define by requiring that the relative changes of the eigenvalues $\epsilon_i$ satisfy

$$\max\left(\left|\frac{\delta\epsilon_i}{\epsilon_i}\right|\right) < \Delta, \tag{35}$$

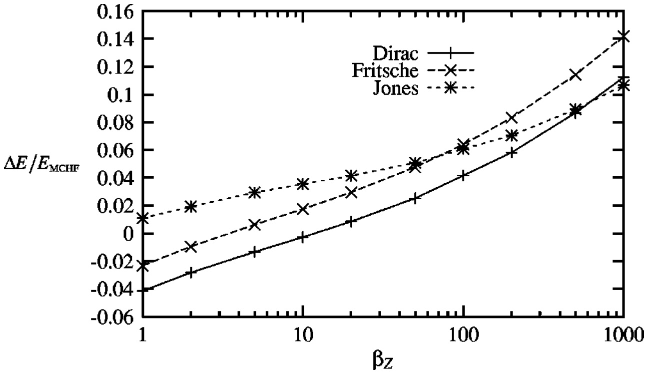

FIG. 3. As in Fig. 1 but for the $|(0,0)(-2,0)\rangle$ state of helium.

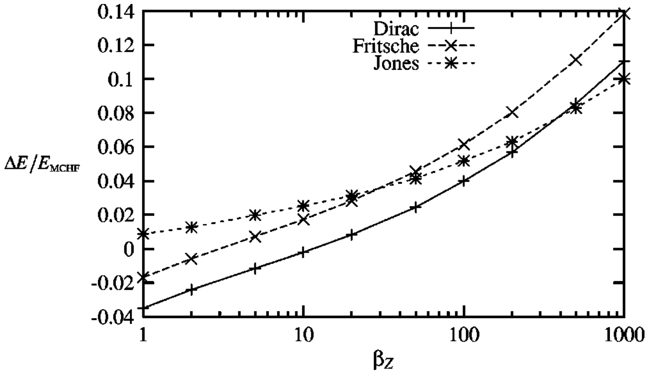

FIG. 4. As in Fig. 1 but for the $|(0,0)(-2,1)\rangle$ state of helium.

where $\Delta=10^{-5}$. To speed up our calculations, we evaluate the self-consistent potential-terms at the grid points of our finite-element grid and interpolate the potential with the same basis that is used for the wave functions. Once self-consistency is reached for a value of $Z>n_e$, another iteration for $Z:=Z-1$ can be done. This will be necessary for convergence in cases where neutral or nearly neutral atoms are to be calculated, since an attempt to calculate the system starting with $Z=n_e$ will often, especially for $Z\gtrsim 10$, not converge.

## V. RESULTS

For helium and heliumlike atoms in very strong magnetic fields, there are quite a number of atomic data results in the literature [4,6,7,13] and it is thus the natural starting point for a comparison. For heavier atoms there are also some results available [12,11,22], but most of them only consider ground states.

### A. Ground-state energies

In Table I, we show the ground-state energies obtained for helium for a wide range of values of $\beta_Z$ using the functionals due to Dirac, Fritsche, and Jones. For comparison, the extrapolated results of a multi-Landau-channel Hartree-Fock (MCHF) calculation [6] are also shown. It is evident, that the density-functional calculations agree reasonably well with the HF-results for $\beta_Z\lesssim 100$, but give much more binding for $\beta_Z\gtrsim 100$. For $\beta_Z<200$, the density-functional results decrease from left to right. In Fig. 1, the relative deviation of the density-functional results from the MCHF results is shown as function of $\beta_Z$. It is seen that the degree of overbinding increases with $\beta_Z$ for all functionals considered. In addition, it is clear from both the table and the figure, that the functional due to Jones performs best at small $\beta_Z$ values, the one due to Fritsche gives a better performance for moderately large values of $\beta_Z$, while the functional due to Dirac binds slightly less strongly than and shows a nearly constant distance from the one due to Fritsche, which is not surprising since they only differ by a factor, and all functionals overbind very strongly at very large values of $\beta_Z$. We have not yet found an explanation for this behavior.

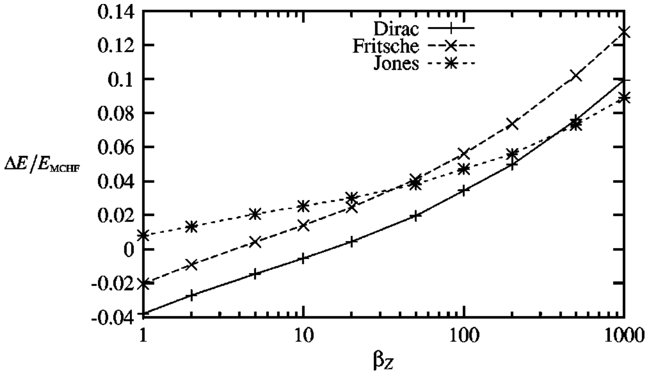

FIG. 5. As in Fig. 1 but for the $|(0,0)(-3,0)\rangle$ state of helium.

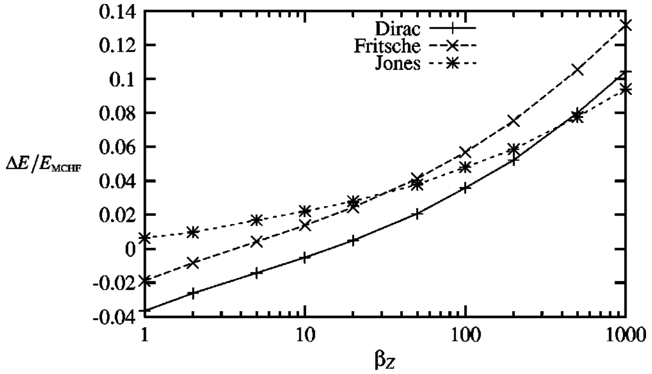

FIG. 6. As in Fig. 1 but for the $|(0,0)(-3,1)\rangle$ state of helium.

In Table II, we show the ground-state energies obtained with the functional due to Jones for helium, carbon, and neon at magnetic-field values, for which density-functional calculations have previously been done. We obtain slightly more binding, since the results in the literature were done in the adiabatic approximation, i.e., using only one Landau channel. This is especially true for $Z=10$, where $\beta_Z$ is smaller and thus the higher Landau channels will be more important.

In Table III we show the results obtained for the ground-state energies of carbon $(Z=6)$ and neon $(Z=10)$ in very strong magnetic fields using the functional due to Fritsche on the same $\beta_Z$ grid as used for helium. Due to the lack of prior calculations in this field, it is admittedly difficult to estimate the accuracy of our results obtained for those atoms. Based on the above comparison for helium with MCHF calculations, we extrapolate that these results should have an accuracy of about 3 to 5%.

### B. Energies of excited states

For the excited states $|(0,0)(-1,1)\rangle$, $|(0,0)(-2,0)\rangle$, $|(0,0)(-2,1)\rangle$, $|(0,0)(-3,0)\rangle$, and $|(0,0)(-3,1)\rangle$ of helium, we show in Tables IV–VIII, the results obtained for the same functionals as in Table I in comparison to the extrapolated HF-calculations. In Figs. 2–6, we also show the relative energy differences as in Fig. 1 as a function of the magnetic field. The deviation of the density-functional results from our MCHF values shows a similar behavior as for the ground state except that the intercept between results for the Fritsche and Jones functionals happens at a smaller value of $\beta_Z$; again for $\beta_Z\lesssim 100$ the functional due to Fritsche seems on average to be the best choice among the three considered.

Since we expect the main applications of our results to be in the region $1 \lesssim \beta_Z \gtrsim 100$, we will, in future, use the functional due to Fritsche for our calculations.

## VI. SUMMARY

We have shown, how the method of finite elements and the density-functional approach can be combined to yield results for atoms in very strong magnetic fields, that should be sufficiently accurate for the application in neutron star spectroscopy. It has also been demonstrated, that the functional due to Fritsche, which is derived from the assumption of a Gaussian correlation factor seems to be the best choice for $1 \lesssim \beta_Z \lesssim 100$. An additional advantage of this functional is that it can be improved upon in a systematic manner by determining the width of the Gaussian self-consistently from the density. This method was applied to atoms in the field-free case by Cordes and Fritsche [23], who report results that are quite close to Hartree Fock, while still retaining most of the advantages of the density-functional approach. Investigations in this regard are planned. In a forthcoming paper we plan to give results for the oscillator strengths of selected dipole transitions for some multielectron atoms in strong magnetic fields.

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