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Multichannel density-functional calculations for atoms and atomic chains in magnetic fields of compact stars

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Ground-state energies of atoms and atomic chains in strong to superstrong magnetic fields ($B \approx 2.4\times10^6$ – 8.5×10^8 T) are calculated within the single-particle scheme of a heuristic density-functional method. From these we find condensation energies and binding lengths. Using the local Dirac exchange functional, the corresponding equations are solved iteratively, expanding the wave functions with respect to Landau functions in the transverse directions and directly integrating along the longitudinal direction. Dropping the adiabatic approximation, we extrapolate our results with respect to the number of Landau channels taken into account. The values found by this extrapolation correspond to calculations without any restriction on the allowed wave functions. [S1050-2947(96)11106-9]

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I. INTRODUCTION

Since the discovery of huge magnetic fields in the vicinity of compact cosmic objects, i.e., white dwarfs ($B\approx10^2$–10^5 T; Ref. [1]) and neutron stars ($B\approx10^7$–10^9 T; Ref. [2]), the study of properties of matter in such fields has — despite many impressive successes [3] — not yet yielded reliable results as to deciding on its actual state. The question of condensation of matter in these fields plays an important role in interpreting observed spectra of compact cosmic objects and in modeling their magnetospheres. Due to the extreme anisotropy caused by the magnetic field, there is evidence that the condensation of matter, which has to happen in some three-dimensional lattice, can already be assessed by looking at (weakly interacting) linear atomic chains oriented along the field lines. The weak (quadrupole-quadrupole) interaction does not need to be included in a fully self-consistent solution of the problem but can be treated as a small perturbation afterwards.

In this work, we present results of self-consistent calculations for many-particle systems in strong and superstrong magnetic fields that take into account more than the lowest Landau level and go beyond Thomas-Fermi calculations [4]. Extrapolating from our results for finite numbers of Landau levels, we find for a wide range of magnetic field strengths condensation energies and binding lengths for atomic chains without any restriction on the allowed wave functions.

The physical theory applied is a simple heuristic density-functional method. We obtained the corresponding single-particle equations from the Kohn-Sham equations of spin-density-functional theory (SDFT) by adding the term representing the coupling between the electrons and the vector potential to the operator of the canonical momentum in the kinetic energy term. In the exchange-correlation functional, we make use of the local-density approximation (LDA).

II. METHOD

Using cylindrical coordinates (ϱ,φ,z) and choosing the z axis parallel to the homogeneous magnetic field, we expand our equations in terms of Landau functions in the axially symmetric gauge, $\mathbf{A}(\mathbf{r})=\frac{1}{2}\mathbf{B}\times\mathbf{r}$, for the vector potential,

$$\Phi_{n_L m}(\varrho,\varphi)=\frac{1}{a_L\sqrt{\pi}}e^{im\varphi}I_{n_L s}(\varrho^2/a_L^2), \tag{2.1}$$

which are characterized by the Landau quantum number n_L and the z component m of the orbital angular momentum. Here we have $s=n_L-m\geqslant0$, the Larmor radius $a_L=\sqrt{2\hbar/eB}$,

$$I_{ns}(\xi)=(-1)^s(n!s!)^{-1/2}e^{-\frac{\xi}{2}}\xi^{(n-s)/2}Q_s^{n-s}(\xi), \tag{2.2}$$

and Q_s^{n-s}, the generalized Laguerre polynomial of degree s. We arrive at a system of one-dimensional integro-differential equations for the longitudinal functions $f_{n_L mk}$,

$$-\frac{\hbar^2}{2m_\mathrm{e}}f''_{n_L mk}(z)+\sum_{n'_L=0}^{n_\mathrm{max}}V^{n_L n'_L m}(z)f_{n'_L mk}(z)+\left[\left(n_L+\frac{1}{2}\right)\hbar\omega_c-\varepsilon_{n_L mk}\right]f_{n_L mk}(z)=0. \tag{2.3}$$

Imposing cyclic boundary conditions, its solutions give single-particle wave functions of the Bloch type,

$$\psi_{mk}(\varrho,\varphi,z)=\sum_{n_L=0}^{n_\mathrm{max}}f_{n_L mk}(z)\Phi_{n_L m}(\varrho,\varphi), \tag{2.4}$$

characterized by some wave number k. We omit an index at the functions ψ and f, which refers to the zone number, the analog to the number of nodes in the z direction in the case of wave functions of single atoms. This number can take on non-negative integer values but is fixed to 0 in our calculations. This is a restriction neither for hydrogen at any magnetic flux density nor for light elements at the magnetic flux densities considered here. The corresponding energy bands cannot be populated for hydrogen where we need to fill up only a k-space ''volume'' of $2\pi/a$. For the light elements

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and magnetic flux densities considered here, the states in these bands have too high energies to be populated. In Eq. (2.3), $\omega_c = eB/m_e$ is the cyclotron frequency; the one-dimensional effective potentials are given by

$$V^{n_L n'_L m}(z) = \int_0^\infty \int_0^{2\pi} \Phi^*_{n_L m}(\varrho,\varphi) V_{\mathrm{eff}}(\varrho,z) \times \Phi_{n'_L m}(\varrho,\varphi) d\varphi \varrho \, d\varrho, \tag{2.5}$$

while

$$V_{\mathrm{eff}}(\varrho,z) = V(\varrho,z) + V_{\mathrm{H}}(\varrho,z) + V_{\mathrm{xc}}(\varrho,z) \tag{2.6}$$

consists of the external potential V, the direct part V_{H} of the electron-electron potential, and its exchange-correlation part

$$V_{\mathrm{xc}}(\varrho,z) = \frac{\delta E_{\mathrm{xc}}[n]}{\delta n(\varrho,z)}. \tag{2.7}$$

Within the LDA where

$$E_{\mathrm{xc}}^{\mathrm{LDA}}[n] = 2\pi \int n(\varrho,z) \varepsilon_{\mathrm{xc}}(n(\varrho,z)) \varrho d \varrho dz, \tag{2.8}$$

we use the simple Dirac exchange functional

$$\varepsilon_{\mathrm{x}}(n) = -\frac{3}{2} \frac{e^2}{8\pi\varepsilon_0} \left(\frac{6n}{\pi}\right)^{1/3} \tag{2.9}$$

for the fully polarized electron gas, neglecting correlation effects. For the numerical treatment of the integrals appearing in (2.5), see Pröschel *et al.* [5]. The differential equation solver applied to the system (2.3) of equations, which couples different Landau channels, is based on the one developed by Wintgen [6] for the hydrogen atom in strong magnetic fields.

The equations are solved iteratively using up to three Landau channels [$n_{\max} = 0,1$, or 2 in (2.3) and (2.4)] and simulating continuous occupation of the energy bands up to some common (quasiparticle) Fermi energy ε_{F} by selecting in each (partly) occupied band n_k one-particle states corresponding to equidistant k-values within the interval $[0,k_{\mathrm{F}}^m]$. Here, k_{F}^m is the Fermi wave number of the band characterized by a specific value of m. Iterations are repeated until self-consistency is achieved, i.e., the Euclidean norm of the difference of wave functions obtained in subsequent iterations falls below a given limit.

III. RESULTS

We performed such iterative calculations for infinitely extended linear chains of hydrogen, helium, and carbon atoms. In the case of hydrogen, we considered magnetic field strengths corresponding to 81 different values for the magnetic field parameter $\beta = B/B_0$ with $B_0 \approx 4.70108 \times 10^5$ T. At the magnetic flux density B_0, we have $a_L = a_{\mathrm{Bohr}}$. Within a range from 5 to 1000, the values of β were chosen approximately equidistant on a logarithmic scale. As we also considered elements with nuclear charges $Z > 1$, it is useful to introduce the Z-scaled magnetic field parameter $\beta_Z = \beta/Z^2$.

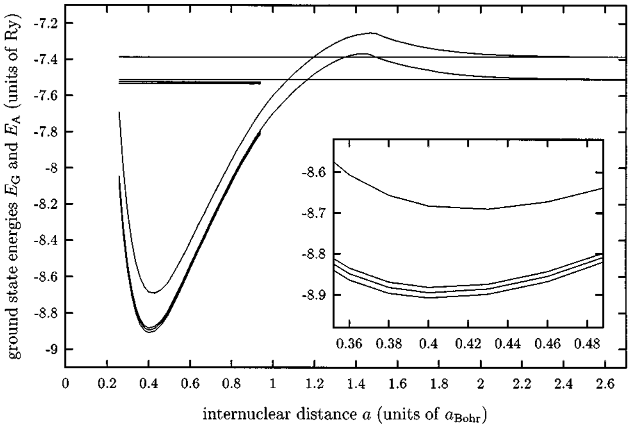

FIG. 1. Ground-state energy $E_G^{[n_{\max}]}(a)$ of a hydrogenic chain at $\beta = 50$. Curves for $n_{\max} = 0,1,2$ and $n_{\max} \to \infty$ are shown. The larger the $n_{\max}$ the lower the corresponding curve. The horizontal lines mark the ground-state energy $E_A^{[n_{\max}]}$ of a hydrogen atom at $\beta = 50$ for $n_{\max} = 0,1,2$ and $n_{\max} \to \infty$, each within the same range of values of a as the corresponding curve for the chain.

In the case of helium, we limited our calculations to $\beta_Z = 50$ ($B \approx 9.4 \times 10^7$ T) and $\beta_Z \approx 265.9$ ($B = 5 \times 10^8$ T); for carbon, to $\beta_Z = 50$ ($B \approx 8.5 \times 10^8$ T) and, in addition, to $n_{\max} = 0$. For $\beta_Z = 50$ and $\beta_Z \approx 265.9$, ground-state energies per atom E_G were obtained in a wide range of internuclear spacings a leading to binding lengths a_0 and binding energies $E_0 = E_G(a_0)$. For other values of β_Z, we restricted our calculations to the regions around a_0. This was possible, since our program for atomic chains allows during one run the variation of β_Z with automatic search for the minimum of E_G as a function of a for each value of β_Z. Condensation energies were found, subtracting binding energies from the ground-state energies E_A of the corresponding single atoms obtained within the same heuristic scheme. These had been already partly calculated by Bühler [7] and were calculated here for hydrogen at several additional values of β.

We examined the convergence of the ground-state energies with the number n_k of single-particle states taken into account in each energy band [8]. These energies are converged with a tolerance of less than 1% when using $n_k = 4$ for the hydrogenic and helium chains and, due to the much larger number of populated energy bands, $n_k = 3$ for carbonic chains. For example, in the case of the hydrogenic chain at $\beta = 50$ ($B \approx 2.35 \times 10^7$ T), increasing n_k from 4 to 5 and 10 increases the binding energy by 0.1% and 0.25%, respectively.

Figure 1 shows for a hydrogenic chain at $\beta = 50$ the resulting ground-state energy $E_G^{[n_{\max}]}(a)$ for $n_{\max} = 0,1$, and 2. In addition, it shows $E_G^{[n_{\max} \to \infty]}(a)$, where the extrapolation with respect to the highest allowed Landau quantum number $n_{\max}$ was done assuming a dependence of E_G on $n_{\max}$, which can be expressed as a broken rational function,

$$E_G^{[n_{\max}]} = \frac{a + b(n_{\max}+1)}{1 + c(n_{\max}+1)}. \tag{3.1}$$

Binding energies E_0 and binding lengths a_0 were found for each β_Z from the three deepest fully self-consistently

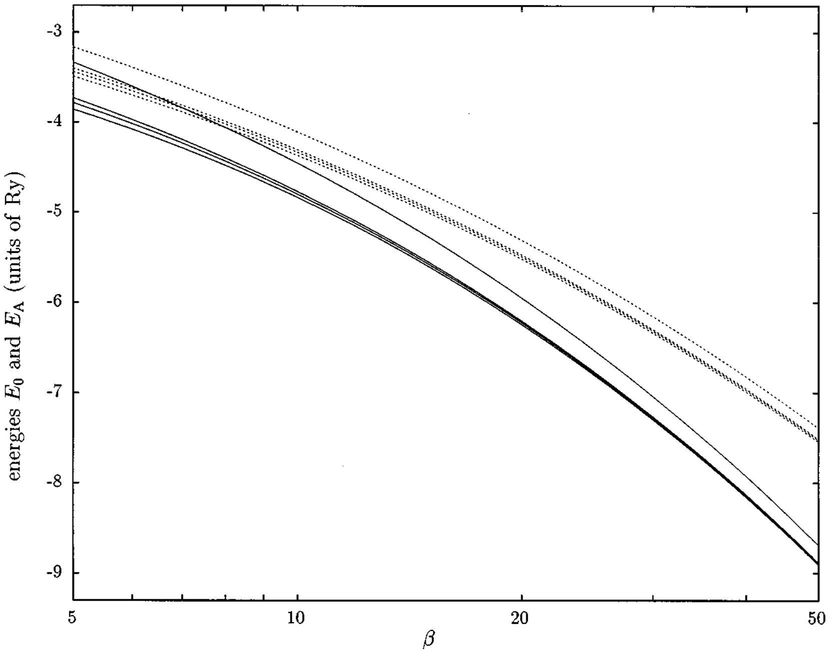

FIG. 2. Binding energy $E_0^{[n_{\max}]}(\beta)$ of a hydrogenic chain (solid lines) and ground-state energy $E_A^{[n_{\max}]}(\beta)$ of a hydrogen atom (dotted lines) for values of β between 5 and 50. Curves for $n_{\max}=0,1,2$ and $n_{\max}\to\infty$ are shown for both cases. The larger the $n_{\max}$ the lower the corresponding curve.

calculated values $E_G(a_i)$ and their corresponding a_i ($i=1,2,3$), assuming a harmonic functional dependence of E_G on a in the region around its minimum E_0. For hydrogen at $5\leq\beta\leq 1000$, $E_0^{[n_{\max}]}$ and $E_A^{[n_{\max}]}$ are plotted in Figs. 2 and 3 for $n_{\max}=0,1,2$ and for $n_{\max}\to\infty$. The binding lengths decrease when dropping the adiabatic approximation, i.e., when allowing for $n_{\max}>0$.

The ground-state energies of single atoms and of atomic chains also decrease when $n_{\max}$ is increased. As a net effect, the condensation energy $E_C=E_A-E_0$ increases in all cases examined here. For hydrogen at $5\leq\beta\leq 1000$, this is shown in Fig. 4. Figure 5 shows the corresponding binding lengths. The self-consistent calculations with $n_{\max}>0$ were performed for chains at $\beta=5$, 10, 20, 50, 100, 200, 500, and 1000 only. Within this range, E_G, E_C, and a_0 at arbitrary values were then found by interpolation applying a natural cubic spline.

$E_G^{[n_{\max}]}(a)$ for a helium chain at $\beta_Z=50$ is plotted together with $E_A^{[n_{\max}]}$ for the helium atom using $n_{\max}=0,1,2$ and for $n_{\max}\to\infty$ in Fig. 6. For $Z>1$, we use Z-scaled atomic units, i.e., $a_Z=a_{\rm Bohr}/Z$ and $E_Z=Z^2$Ry. $E_G^{[n_{\max}=0]}(a)$ for a carbonic chain at $\beta_Z=50$ is plotted together with $E_A^{[n_{\max}=0]}$ for the carbon atom in Fig. 7. Both of these two atomic chains exhibit a relative minimum of $E_G(a)$; in the case of carbon, at an internuclear distance very close to a_0. Between

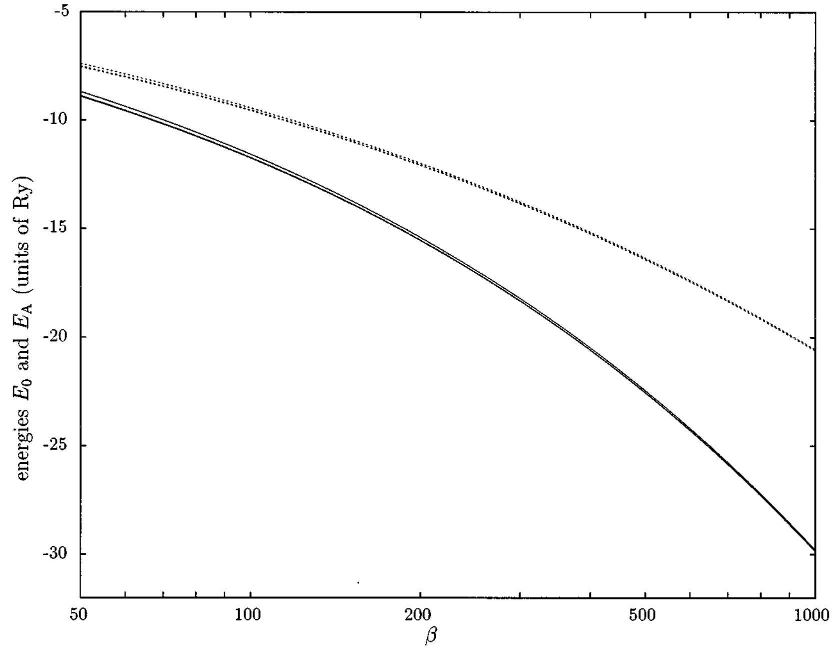

FIG. 3. Same as Fig. 2, but for values of β between 50 and 1000.

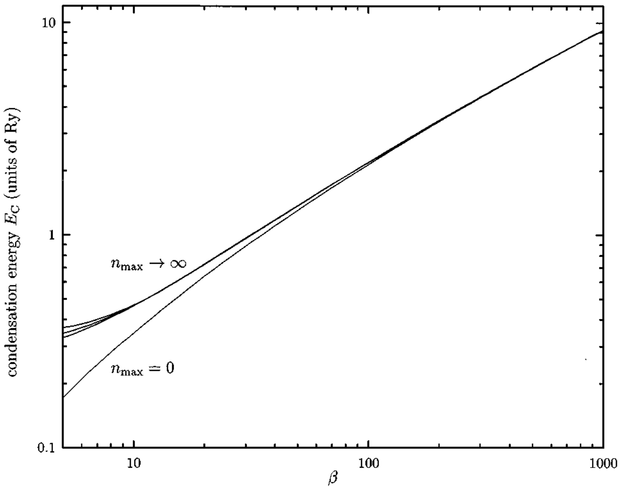

FIG. 4. Condensation energy $E_C^{[n_{\max}]}(\beta)$ of a hydrogenic chain for $n_{\max}=0,1,2$ and $n_{\max}\to\infty$.

such a minimum and the corresponding relative maximum of $E_G(a)$, a new energy band starts to be populated, if a is decreased.

For large internuclear distances, the overlap of the electronic charge densities of the individual atoms within an atomic chain is negligible, and the atoms interact only via their quadrupole moments. For an atomic chain, the energy shift caused by this quadrupole-quadrupole interaction is given by

$$\Delta E^Q = \frac{3e^2}{8\pi\varepsilon_0}\frac{Q_{zz}^2}{a^5}\sum_{i=1}^{\infty}\frac{1}{i^5}, \tag{3.2}$$

where the deviation of the factor $\Sigma_{i=1}^{\infty} i^{-5} \approx 1.037$ from 1 is due to the contributions of interactions between atoms that are not next neighbors. For our calculations at $\beta_Z=50$, the values we find in the repulsive region for $Q_{zz}=2\langle z^2\rangle - 2\langle x^2\rangle$ are listed in Table I.

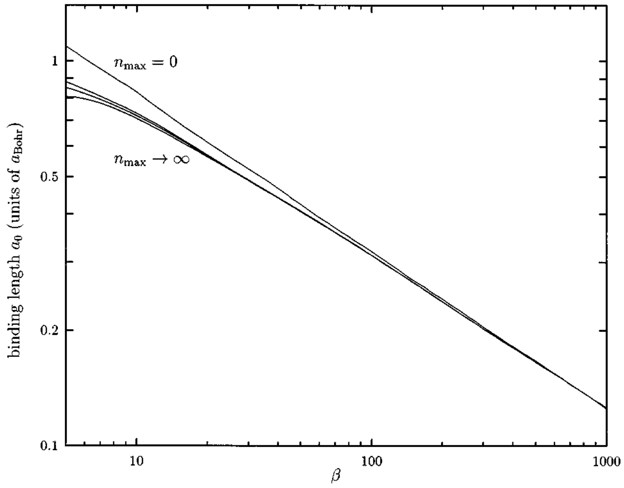

FIG. 5. Binding length $a_0^{[n_{\max}]}(\beta)$ of a hydrogenic chain for $n_{\max}=0,1,2$ and $n_{\max}\to\infty$.

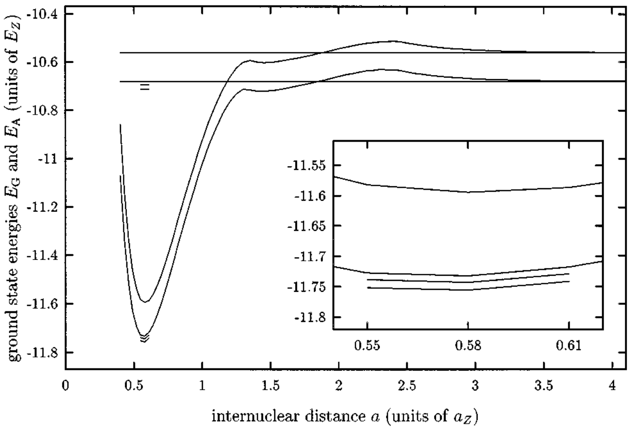

FIG. 6. Same as Fig. 1, but for helium at $\beta_Z=50$.

IV. COMPARISON WITH REPORTED RESULTS

Our results for the ground-state energies E_A of single atoms, binding energies E_0 of atomic chains, condensation energies E_C, binding lengths a_0, and the values $m_{\max}$ of the z component m of the orbital angular momentum of the highest occupied quasi-single-particle states at a_0 are compiled in Table II for hydrogen and in Table III for helium as well as carbon, together with those of other authors for some values of β_Z that they considered.

The ground-state energies obtained by Ruder *et al.* [3] are the most accurate ones available today for single atoms. Table II gives, separated by a slash, upper and lower limits to the true values for these energies. These results can be used to assess the accuracy of the different approximating schemes when applied to single atoms. As these are obtained without any restriction on the allowed wave functions, we also list our corresponding results for $n_{\max}\to\infty$.

All other values listed in Tables II and III were calculated within the adiabatic approximation. Abrahams and Shapiro [9] employed a Thomas-Fermi-Dirac-Weizsäcker statistical model in which the magnetic Thomas-Fermi-Dirac kinetic, potential, and exchange energy functionals are supplemented

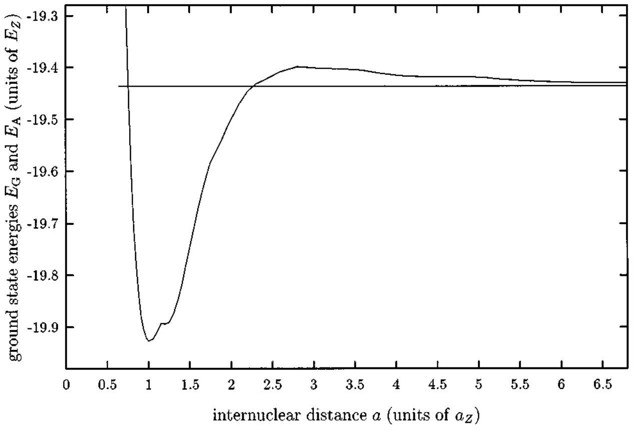

FIG. 7. Ground-state energy $E_G^{[n_{\max}=0]}(a)$ of a carbonic chain at $\beta_Z=50$. The horizontal line marks the ground-state energy $E_A^{[n_{\max}=0]}$ of a carbon atom at $\beta_Z=50$.

TABLE I. Quadrupole moment component Q_{zz} in units of $a_Z^2 = a_{\mathrm{Bohr}}^2/Z^2$ for atoms with nuclear charge Z within atomic chains at large internuclear distances a (repulsive region) in magnetic fields corresponding to the value $\beta_Z = 50$ for the Z-scaled magnetic field parameter.

Z	Q_{zz}
1	0.255
2	1.1
6	6.7

by a gradient correction to the kinetic energy. Müller [10] applied a variational method within the Hartree-Fock approximation and divided, for the modeling of atomic chains, electrons into ''core'' and ''sheath'' electrons. The interaction between these two kinds of electrons was approximated by effective charges of the nuclei. Neuhauser, Koonin, and Langanke [11], Lai, Salpeter, and Shapiro [12], as well as Demeur, Heenen, and Godefroid [13] used the unrestricted Hartree-Fock method directly, which can be applied with present computer resources only to single atoms or — as in Refs. [12,13] — to finite chains. The results of Demeur, Heenen, and Godefroid [13] given in Table II are actually for the H_5 molecule, but appear to be already stabilized when compared with the results for H_i $(i = 2,3,4)$ also presented in their paper. Because of the numerical complexity of this unrestricted Hartree-Fock method when applied to many-electron systems, Refs. [11,12] also had to retreat on variational calculations for infinite chains. Neuhauser, Koonin, and Langanke [11] restricted the longitudinal single-particle wave functions to products $u_m(z)e^{ikz}$ of plane waves and k-independent periodic functions with period a; and Lai, Salpeter, and Shapiro [12], simply to plane waves.

Despite the fact that the Hartree-Fock approximation gives, in general, better results for single atoms than density-functional methods applying the LDA, this superiority is easily destroyed by the further approximations that are neccessary for extended systems. The order of magnitude of the effect of restrictions imposed on the wave functions on the ground-state energy can be seen from the two values for E_A of a helium atom at $\beta_Z \approx 53.18$ ($B = 10^8$ T) calculated by Müller [10] and by Neuhauser, Koonin, and Langanke [11],

TABLE II. Ground-state energy E_A of hydrogen atoms, binding energy E_0 of hydrogenic chains, condensation energy E_C, binding length a_0, and the value $m_{\max}$ of the z component of the angular momentum of the highest occupied single-particle state in magnetic fields corresponding to the magnetic field parameter β from calculations allowing the maximum Landau quantum number $n_{\max}$. We use atomic units, rydbergs, and a_{Bohr}, and compare our results with those of other authors. (Slashes separate upper and lower limit of the true values.)

	β	$n_{\max}$	E_A	E_0	E_C	a_0	$m_{\max}$
	20	0	−5.308	−5.946	0.637	0.614	−3
	20	→∞	−5.516	−6.241	0.725	0.563	−3
RWHG [a]	20	→∞	−5.602058/60				
	21.2717	0	−5.429	−6.100	0.671	0.599	−3
LSS [b]	21.2717	0	−5.613	−5.809	0.196	0.58	
	100	0	−9.431	−11.58	2.14	0.320	−5
	100	→∞	−9.554	−11.75	2.19	0.313	−5
RWHG [a]	100	→∞	−9.4531/50				
	106.359	0	−9.635	−11.87	2.24	0.313	−5
LSS [b]	106.359	0	−9.570	−10.77	1.20	0.31	
	200	0	−11.98	−15.40	3.42	0.241	−5
	200	→∞	−12.08	−15.54	3.46	0.237	−5
RWHG [a]	200	→∞	−11.7023/39				
	212.717	0	−12.24	−15.80	3.56	0.235	−6
AS [c]	212.717	0			2.94	0.206	
LSS [b]	212.717	0	−11.87	−13.99	2.12	0.23	
	425.434	0	−15.48	−21.00	5.52	0.177	−7
LSS [b]	425.434	0	−14.59	−18.15	3.56	0.17	
	500	0	−16.34	−22.43	6.10	0.166	−7
	500	→∞	−16.41	−22.54	6.13	0.165	−7
RWHG [a]	500	→∞	−15.3241/53				
DHG [d]	500	0	−15.2	−18.8	3.6	0.17	−3
	1000	0	−20.56	−29.80	9.23	0.126	−8
	1000	→∞	−20.62	−29.88	9.26	0.125	−8
RWHG [a]	1000	→∞	−18.60896/986				
LSS [b]	1063.59	0	−18.90	−25.56	6.66	0.12	

[a] Ruder *et al.* [3].

[b] Lai, Salpeter, and Shapiro [12].

[c] Abrahams and Shapiro [9].

[d] Demeur, Heenen, and Godefroid [13].

TABLE III. Same as Table II, but for helium and carbon. We use Z-scaled atomic units, i.e., $E_Z=Z^2$Ry and $a_Z=a_{\mathrm{Bohr}}/Z$.

	Z	β_Z	$n_{\max}$	E_A	E_0	E_C	a_0	$m_{\max}$
	2	50	0	−10.56	−11.59	1.03	0.583	−8
	2	50	→∞	−10.71	−11.75	1.04	0.572	−8
RWHG [a]	2	50	→∞	−10.36				
AS [b]	2	53.1793	0	−9.00	−10.29	1.29	0.51	
M [c]	2	53.1793	0	−10.01	−10.93	0.92	0.550	−6
NKL [d]	2	53.1793	0	−10.57	−11.03	0.46	0.58	
	2	265.896	0	−18.77	−22.81	4.04	0.293	−12
J [e]	2	265.896	0	−19.11	−23.16	4.05	0.29	
J [e]	6	29.5440	0	−16.4	−16.6	0.2	1.35	
	6	50	0	−19.44	−19.93	0.49	1.014	−22

[a] Ruder *et al.* [3].
[b] Abrahams and Shapiro [9].
[c] Müller [10].
[d] Neuhauser, Koonin, and Langanke [11].
[e] Jones [14].

respectively, listed in Table III. Müller [10] allowed only for in the z direction exponentially decaying wave functions with no or one node. The unrestricted result of Neuhauser, Koonin, and Langanke [11] is lower by 5.5%. As in both papers similar variational Hartree-Fock-like approaches are chosen for atomic chains, the values for E_0 differ only by 0.9%. But the condensation energies differ by 50%. For the chains, such Hartree-Fock-like calculations give weaker binding, i.e., condensation energies that are smaller than the ones we found. The differences in E_C for hydrogen increase, for example, if compared with the results of Lai, Salpeter, and Shapiro [12] from about 30% for the largest magnetic fields considered here to 71% at $\beta\approx 21.27$.

Our condensation energies and binding lengths can be compared quite directly with the results of similar density-functional calculations by Jones [14–16] for atomic chains and lattices. The local exchange-correlation functional applied in those papers reads

$$\varepsilon_{\mathrm{xc}}^{\mathrm{Jones}}(N)=[(13.7-3\pi\ln(2\beta_Z)+2\pi\ln N)\beta_Z^{-1}N \\ -9.45\sqrt{2}\beta_Z^{-5/2}N^2+\{0.0288\ln(2\beta_Z)-0.244 \\ -0.0192\ln N\}\sqrt{2\beta_Z}]\frac{E_Z}{Z}, \qquad (4.1)$$

with $N\equiv na_Z^3$. Using this functional, we were able to reproduce the results of Jones [14] for helium at $\beta_Z\approx 265.9$ in the adiabatic approximation with an accuracy of about 0.25% for E_A and E_0, 0.4% for E_C, and 1.5% for a_0. Using the Dirac exchange functional, we get a very similar value for E_C that differs only by 0.25%, although E_A and E_0 differ by about 2% (see Table III). This shows that the condensation energies are rather insensitive to the actual local exchange-correlation functional used.

V. CONCLUSION AND OUTLOOK

We presented results of multichannel density-functional calculations for matter in astrophysically relevant magnetic fields using a set of Landau functions. In weak neutron star magnetic fields, the effect of higher Landau levels on ground-state energies, condensation energies, and binding lengths is not negligible. Within the heuristic density-functional method applied here, the local exchange-correlation functional actually used has little effect on condensation energies, as differences in ground-state energies largely cancel. Comparision of the condensation energies we find with the ones obtained within other heuristic theories (Thomas-Fermi-like or Hartree-Fock-like) shows much larger differences. These are not only due to the use of different physical theories; they are, in the case of Hartree-Fock-like calculations for chains, also due to restrictions on the allowed single-particle wave functions.

Our calculational scheme is such that it can be easily generalized to an implementation of current-density-functional theory (CDFT) (Vignale and Rasolt [17,18]; Vignale, Rasolt, and Geldart [19]), the only theory available today which — apart from a Monte Carlo treatment of the many-particle Schrödinger equation — in principle can lead to true ground-state energies for many-particle systems in strong magnetic fields. In such a modified scheme, calculations for these systems are only restricted by the quality of the exchange-correlation functional. As additional terms containing gradients enter the Kohn-Sham equations when going from the heuristic density-functional method applied here to CDFT, the condensation energies obtained may be considerably shifted. Therefore, we plan to substitute the method applied in this work by CDFT, which correctly takes into account diamagnetic effects, together with the corresponding exchange-correlation functionals (e.g., Skudlarski [20] and Skudlarski and Vignale [21]).

ACKNOWLEDGMENT

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