

### Hartree-Fock calculations of atoms and molecular chains in strong magnetic fields

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We calculate the binding energies of atoms and molecular chains in  $10^{12}$  G magnetic fields using the Hartree-Fock method. For  $Z > 2$  (4) at  $1 \times 10^{12}$  ( $5 \times 10^{12}$ ) G, the isolated atom is energetically favored over the molecular chain.

Atomic structure in very strong magnetic fields ( $B \equiv 10^{12} B_{12} = 10^{12} - 10^{13}$  G) is of relevance to neutron star studies.<sup>1-3</sup> Of particular importance is the question of whether the surface matter is a solid or isolated atoms. For example, if the cohesive energy of the solid is  $\leq 3$  keV per atom, the surface matter will not support a finite electric-field boundary condition.<sup>4</sup> Models of surface heating by impact of solid matter also depend on whether material will solidify in strong magnetic fields.<sup>5</sup>

In this paper we report the results of variational [Hartree-Fock (HF)] calculations for matter in strong magnetic fields. We calculate the energy of both isolated atoms and linear chains. Our calculations are the first self-consistent ones treating exchange properly for atoms heavier than helium in high fields,<sup>6</sup> and are therefore particularly important for neutron star surfaces, where the dominant material is believed to be iron.

Previous studies of this problem include restricted variational<sup>7</sup> and density-functional calculations,<sup>8</sup> the isolated atom case was also studied using the Thomas-Fermi-Dirac method.<sup>9</sup> However, a more exact treatment is needed to obtain quantitative results, because the errors introduced by these methods are of the same order as the cohesive energy (a few percent of the total energy). The lack of correlations in the Slater determinant that we assume probably underestimates the absolute binding energies by less than 1%.<sup>8</sup> Moreover, since we are interested in the energy difference between the isolated atom and the solid, the deficiencies of the Hartree-Fock method partially cancel.

We assume an isolated linear chain of regularly spaced stationary nuclei (charge  $Z$ , spacing  $a$ ) oriented along the magnetic field (strength  $B$ ). The magnetic field confines the  $Z$  electrons per unit cell to Landau orbitals around the chain, while motion along the chain is governed by the electrostatic interactions among the nuclei and the electrons.

The corrections due to chain-chain interactions are estimated to be less than 1%,<sup>10</sup> and relativistic corrections have been shown to be unimportant for these field strengths.<sup>11</sup> The Hamiltonian therefore can be written as

$$H = H_B + V_{en} + V_{ee} + V_{nn} \quad (1)$$

where  $H_B$  is a one-body Hamiltonian describing the motion of independent electrons in the magnetic field, and  $V_{en}$ ,  $V_{ee}$ , and  $V_{nn}$  are the electrostatic electron-nucleus, electron-electron, and nucleus-nucleus interactions, respectively.

We seek to estimate the lowest eigenvalue of  $H$  as a function of the spacing  $a$  for a given field strength  $B$ . To do so, we assume a determinantal trial wave function formed from spin-aligned single-particle wave functions of the form

$$\psi_{m\nu} = L_{-m_0}(\rho, \phi) e^{ikz} u_{m\nu}(z) |s_z = -\frac{1}{2}\rangle \quad (2)$$

Here,  $(\rho, \phi, z)$  are the usual cylindrical coordinates, the non-negative integer quantum number  $m$  specifies the  $z$  component of orbital angular momentum, and  $\nu$  is the quantum number of motion along the field. The Bloch factor  $e^{ikz}$  with  $|k| \leq \sigma_{m\nu} \pi/a$  is a consequence of the periodicity of the chain. Here,  $0 \leq \sigma_{m\nu} \leq 1$  is the occupation of the  $m\nu$  band.  $L_{-m_0}$  is the Landau orbital that is an eigenstate of  $H_B$  with eigenvalue  $0$ :<sup>12</sup>

$$L_{-m_0}(\rho, \phi) = (2\pi m!)^{-1/2} e^{-im\phi} e^{-\rho^2/4} \quad (3)$$

where we measure all lengths in units of  $\hat{\rho} = (\hbar c/eB)^{1/2} = 2.566 \times 10^{-10} B_{12}^{-1/2}$  cm and where  $B_{12}$  is  $B$  measured in units of  $10^{12}$  G. We approximate the periodic functions  $u_{m\nu}$  as independent of  $k$  and will determine them variationally.

With the wave functions (2), the various terms in the variational energy per unit cell,  $E$ , can be written as

$$\langle H_B \rangle = \frac{\hbar^2}{2m_e} \sum_{m,\nu} \sigma_{m\nu} \left[ \frac{1}{3} \left( \frac{\pi \sigma_{m\nu}}{a} \right)^2 + \int |u'_{m\nu}(z)|^2 dz \right] \quad (4a)$$

$$\langle V_{en} \rangle = - \frac{Ze^2}{\hat{\rho}} \sum_{m,\nu} \sigma_{m\nu} \int V_m(z) |u_{m\nu}(z)|^2 dz \quad (4b)$$

$$\langle V_{ee} \rangle = \frac{e^2}{2\hat{\rho}} \sum_{m,\nu,m',\nu'} \left[ \sigma_{m\nu} \sigma_{m'\nu'} \int \int D_{mm'}(z-z') |u_{m\nu}(z)|^2 |u_{m'\nu'}(z')|^2 dz dz' - \int \int E_{mm'}(z-z') u_{m\nu}(z) u_{m'\nu'}(z') u_{m'\nu'}^*(z) u_{m\nu}^*(z') dz dz' \right] \quad (4c)$$

$$\langle V_{nn} \rangle = \frac{Z^2 e^2}{a\hat{\rho}} \sum_{j=1}^{\infty} \frac{1}{j} \quad (4d)$$

with the periodic nuclear, direct, and exchange kernels:

$$V_m(z) = \sum_{n=-\infty}^{\infty} \int \frac{e^{-\rho^2/2} \rho^{2m+1}}{2^m m! \sqrt{\rho^2 + z_n^2}} d\rho, \quad (5a)$$

$$D_{mm'}(z) = \sum_{n=-\infty}^{\infty} \int \int \frac{e^{-[\rho^2 + (\rho')^2]/2} \rho^{2m} (\rho')^{2m'}}{2^{m+m'} m! m'! \sqrt{(\rho - \rho')^2 + (z_n)^2}} d\rho d\rho', \quad (5b)$$

$$E_{mm'}(z) = \sum_{n=-\infty}^{\infty} \frac{\sin(\sigma_{mv} z_n \pi/a) \sin(\sigma_{m'\nu'} z_n \pi/a)}{(z_n \pi/a)(z_n \pi/a)} \int \int \int \int \frac{e^{-[\rho^2 + (\rho')^2]/2} (\rho \rho')^{m+m'+1} e^{-i(m-m')(\phi-\phi')}}{2^{m+m'} m! m'! \sqrt{(\rho - \rho')^2 + (z_n)^2}} d\rho d\rho' d\phi d\phi'. \quad (5c)$$

Here the integrals in Eqs. (4) run over the unit cell ( $|z| \leq a/2$ ) and  $z_n \equiv z - na$  in Eqs. (5). Note that  $\langle V_{en} \rangle$ ,  $\langle V_{nn} \rangle$ , and the direct part of  $\langle V_{ee} \rangle$  are formally divergent, but can be canceled analytically to give the finite energy of interest.<sup>7</sup>

The Hartree-Fock equations are obtained straightforwardly by varying  $E$  with respect to  $u_{mv}$ . To account for degeneracies in the higher Bloch bands, we determine the  $\sigma_{mv}$  self-consistently by requiring

$$\partial E / \partial \sigma_{mv} = \epsilon_F \quad (6)$$

for the partially occupied bands, where  $\epsilon_F$  is the Fermi energy. The isolated atom is obtained as  $a$  becomes large, in which case our approximation of  $u_{mv}$  as independent of  $k$  becomes exact.

We discretized the Hartree-Fock equations on a uniform mesh spanning the unit cell and solved them by iteration; typically between 64 and 256 points were used. The set of initial single-particle wave functions was obtained from variational calculations,<sup>13</sup> but we checked that the final solution was invariant to wide variations in the initial wave functions.

The kernels (5) are all periodic in  $z$  and so are best dealt with in Fourier space using the fast Fourier transform. The Fourier transform of the electron-nucleus interaction (5a) is proportional to a Whittaker function,<sup>14</sup> which we calculate by Taylor expansion for small  $q$  and by numerical integration for larger  $q$ . The double indexed electron-electron interaction kernels [(5b) and (5c)] can be expressed in terms of a finite sum of the nucleus-electron kernels.<sup>6</sup> However, one complication arises from the Bloch factor in the exchange kernel. We therefore calculate the Fourier

transform of the exchange kernel by convolution in Fourier space using the fact that the Fourier transform of the Bloch factor in Eq. (5c) is a tent function. This allows us to express the Fourier transform of  $E$  as a finite sum of terms of the form

$$\int V_l(Q-q) dq, \quad \int V_l(Q-q) q dq,$$

where the integration limits are linear functions of  $\sigma_{mv}$  and  $\sigma_{m'\nu'}$ . We calculate these integrals by evaluating

$$\int_0^k V_l(q) dq, \quad \int_0^k V_l(q) q dq$$

for a sufficiently fine grid of values of  $k$  and interpolating for each pair of bands  $mv, m'\nu'$ . Numerous checks on our numerical procedures give us confidence in the precision of our results for the total energy to better than  $10^{-3}$ .

Table I shows the energies of isolated helium, carbon, and iron atoms at two magnetic field strengths, together with a comparison to previous calculations, and Table II displays some properties of our iron atom solution. Our results reproduce the helium calculations of Ref. 6. For  $Z=26$  and  $B_{12}=5$ , a combination of the Hartree energy<sup>8</sup> with the exchange energy from variational calculations<sup>7</sup> yield an approximate Hartree-Fock energy of  $-106.18$  keV (Ref. 8), in agreement with our result,  $-106.09$  keV. Our binding energies are slightly lower than those in the density functional calculations. This difference might be attributed to the fact that the exchange functionals in the latter method are approximated using plane waves, which are more appropriate for  $B=0$ , while the Landau orbitals for the present case are actually well localized in the plane perpendicular to the field and do not resemble plane waves.

TABLE I. Absolute values of the ground-state binding energies of atoms as calculated in the Hartree-Fock scheme are compared with density functional (DF) (Ref. 8), density functional with correlations (SIC) (Ref. 8), Thomas-Fermi-Dirac (TFD) (Ref. 9), and restricted variational (RV) (Ref. 7) calculations. Energies are given in keV.

Z	B ( $10^{12}$ G)	HF	DF	SIC	TFD	RV
2	1	0.57532				0.545
	5	0.958	1.040			0.913
6	1	4.230			4.14	
	5	7.668	8.03		7.73	
26	1	55.10	56.1		56.21	53.13
	5	106.09	108.18	108.85	105.89	101.7

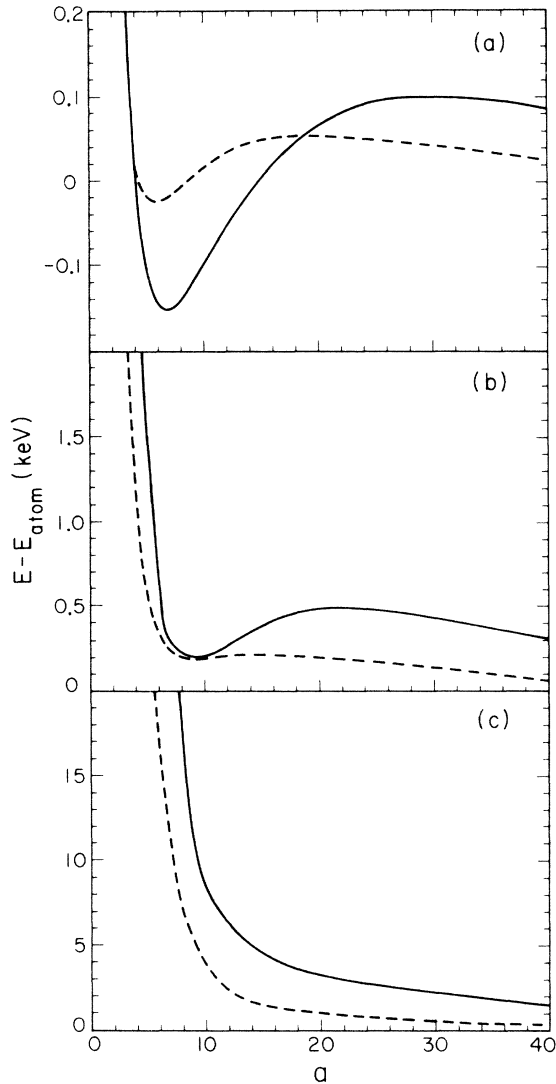


FIG. 1. The ground-state energies per unit cell of infinite linear chains of (a) helium, (b) carbon, and (c) iron are shown as functions of the internuclear separation,  $a$ , for  $B_{12}=1$  (dashed lines) and  $B_{12}=5$  (solid lines). The energies are relative to the isolated atom values. The unit of length for  $a$  is  $2.566 \times 10^{-10} B_{12}^{-1/2}$  cm.

TABLE II. Ionization and  $K$ -shell energies, and the kinetic [Eq. (4a)], nuclear-electron, direct electron-electron, and exchange contributions to the total iron atom energy at  $B_{12}=1$  and 5. The energies are given in keV.

$B$ ( $10^{12}$ G)	$E_i$	$E_K$	$\langle H_B \rangle$	$\langle V_{en} \rangle$	$\langle V_{ee} \rangle$ direct	$\langle V_{ee} \rangle$ exchange
1	0.12	-7.23	10.6	-95.4	32.7	-3.06
5	0.25	-13.86	19.78	-181.7	61.3	-5.41

The energy per unit cell of a chain as a function of the internuclear spacing is shown in Fig. 1. For helium, we have binding, in agreement with the results of Refs. 7 and 8; our binding energies are 25 and 150 eV for  $B_{12}=1$  and 5, respectively. However, for carbon and iron, we do not find binding. Repeating our calculations for  $Z=3-5$ , we find that atoms with  $Z > 2$  (4) are unbound at  $B_{12}=1$  (5). The shapes of the curves agree approximately with the density functional results;<sup>8</sup> the differences again can be attributed to the approximate treatment of the exchange interaction in Ref. 8. However, these differences are of no physical consequences for neutron stars, as they are smaller than 1 keV.

In summary, we have used the Hartree-Fock method to calculate properties of helium and iron in the magnetic fields characteristic of neutron star surfaces. For helium, we find molecular chains energetically favored over isolated atoms, in agreement with previous studies.<sup>7,8</sup> In contrast, for iron we find no binding of the solid. Thus, even if our physical treatment of the problem is not valid in all details, it is difficult to believe that the cohesive energy of iron is large enough in  $10^{12}$ -G fields to affect neutron star surfaces. We expect that our results resolve the confusion surrounding this point.<sup>7,10</sup>

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<sup>12</sup>The spacing between Landau orbitals is  $11.5B_{12}$  keV, so that the higher Landau states will have high  $\langle H_B \rangle$  and are therefore of little importance in the ground-state wave functions.

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<sup>14</sup>Our derivation is based on Eq. (A3) given by Virtamo in Ref. 6, but is too lengthy to be given here.