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Properties of matter in ultrahigh magnetic fields and the structure of the surface of neutron stars

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Abstract. The physical properties of atoms, molecules, and solids in the ultrahigh magnetic fields $B \ge 10^9$ G that are believed to exist on the surface of neutron stars are discussed. In these fields, atoms are strongly deformed and elongated along the magnetic field lines; the binding energy and ionising energy of the atoms are substantially increased and the interatomic interaction is dramatically changed. This strongly modifies the properties of matter at the surface of magnetic neutron stars which are crucial for modelling the pulsar magnetosphere. A scenario for magnetosphere evolution is proposed which suggests free emission for a young pulsar and strong binding of the matter to the surface at a later stage. This latter stage is due to strongly bound chains of alternate heavy atoms and light atoms accreted on the surface of the star.

1. Introduction

1.1 High and ultrahigh magnetic fields

There are a variety of well-known effects of magnetic fields in various areas of physics. A strong magnetic field can

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Received 21 October 1994 Uspekhi Fizicheskikh Nauk **165** (2) 121–142 (1995) Translated by Yu V Morozov; edited by J R Briggs magnetise a piece of metal and influence the electric conductivity of metals or semiconductors. Strong magnetic fields are indispensable if thermonuclear plasma is to be confined and thermally insulated. Magnetic fields are referred to as being strong if their effects bring about marked changes in the properties of matter, e.g. electric conductivity, diffusion, etc. However, the definition of 'strong' magnetic field in all such cases remains obscure. Whether a magnetic field should be considered weak or strong depends on its effect on the system and its characteristic parameters, that is, density, temperature, etc. For example, the effect of magnetic field on a ferromagnet is a collective effect that is dependent on a large number of elementary magnetic moments.

Magnetic field effects on electric and thermal conductivity, diffusion, and other kinetic parameters, are identified by minor deviations from equilibrium. For instance, the effect of magnetic field on plasma transport coefficients depends on the ratio of electron collision frequency v_e to the Larmor frequency of electron rotation in a magnetic field

$$\omega_{\rm c} = \frac{eB}{m_{\rm e}c} \approx 1.76 \times 10^7 B \; .$$

In the case of plasma, the magnetic field may be regarded as strong if $v_e/\omega_c \ll 1$. Taking into account the electron collision frequency in a totally ionised plasma

$$v_{\rm e} = \frac{4\sqrt{2\pi}e^4 Z^2 n_i \Lambda}{3\sqrt{m_{\rm e}} T_{\rm e}^{3/2}} = 2.85 \times 10^{-5} \frac{\Lambda}{10} \frac{Zn_i}{T_{\rm e}^{3/2}},$$

where Z is the ion charge and Λ is the Coulomb logarithm, one can obtain the following condition for the strong

magnetic field:

$$B \ge 1.6 \times 10^{-12} \frac{\Lambda}{10} \frac{Zn}{T_{2}^{3/2}}$$

In this expression and those below, temperature is given in electron-volts, magnetic field in Gauss, and density in cm⁻³ (if not stated otherwise). Therefore, given typical parameters of the laboratory thermonuclear plasma (i.e. $n \sim 10^{16} \text{ cm}^{-3}$, $T \approx 5 \text{ keV}$), 'strong' magnetic fields are those of the order of 10 kG, whereas in the case of cosmic interstellar plasma, even magnetic fields of the order of 1 G should be regarded as very strong.

It should be emphasised that it is impossible to develop an absolute classification of the strength of magnetic fields in the framework of classical physics. Such a classification is only feasible in quantum physics where it follows from the comparison between the magnetic moment energy

$$\mu B = \frac{e\hbar}{2m_{\rm e}c}B$$

and the characteristic energy of the system or the particle. Magnetic field which affects spin orientation of electrons or

atoms in a gas with temperature T is defined by the condition

$$\mu B \gg k_{\rm B} T$$
, or $B/G \gg 1.49 \times 10^4 T/{\rm K}$. (1.1)

Magnetic fields in which the energy of a magnetic moment μB is higher than the characteristic binding energy of atoms or molecules (of the order of $Ry \equiv m_e e^4/2\hbar^2$), that is fields such that

$$B > B_9 \equiv \frac{m_e^2 e^3 c}{\hbar^3} = 2.35 \times 10^9 \text{ G} , \qquad (1.2)$$

markedly influence the atomic and molecular structures and their binding and ionisation energies. In a magnetic field such that the radius of the electron orbit for the lowest Landau level $\rho_0 = (\hbar c/eB)^{1/2}$ is less than the Compton length of the electron wave, that is if the condition

$$\mu B > m_{\rm e}c^2$$
, $B > B_{13} \equiv \frac{m_{\rm e}^2 c^3}{e\hbar} = 4.4 \times 10^{13} \,\,{\rm G}$, (1.3)

is satisfied, relativistic effects become important. A magnetic field $B \ge B_{13}$ has a marked effect on the propagation of electromagnetic waves in vacuum: vacuum is polarised, while electrodynamics in such magnetic fields becomes nonlinear. Relativistic effects in magnetic fields $B \ge 10^{13}$ G (specifically the effect of a strong magnetic field on β -decay and inverse β -decay, i.e. electron capture by the nucleus) have been examined in Ref. [1]. Effects of such a field on the neutrino flow emitted by a neutron star appear to be of special interest [2].

Further discussion will be limited to nonrelativistic effects and events in ultrahigh magnetic fields which are characteristic of neutron stars. In other words, we shall proceed from the assumption that $B_{13} > B \ge B_9$. Note that $B_{13} = \alpha^{-2}B_9$, where $\alpha = e^2/\hbar c$ is the fine structure constant.

The objective of the present review is to examine the physical properties of matter in the ultrahigh magnetic fields usually generated at the surface of neutron stars, on the assumption that the magnetic fields satisfy inequality (1.2). In such magnetic fields, the distance between Landau levels is significantly greater than the energy of the Coulomb interaction between electrons and nuclei. Electron shells undergo complete restructuring, atoms take the shape of thin tubules stretched parallel to the magnetic field

lines, and electron spins are oriented strictly against the magnetic field. Specific features of the interaction between completely polarised and grossly deformed atoms account for the creation of matter with significantly new and unusual properties. Depending on the quantum state of the atoms (i.e. ground or weakly excited state), they may exhibit either weak interaction leading to the formation of a Bose-condensate and transition to superfluidity, or strong interatomic interaction which is sufficient to form long polymeric chains of molecules and crystals with high binding energy.

It should be emphasised that Bose condensation is theoretically feasible for spin-polarised hydrogen [3-5] provided inequality (1.1) is satisfied. Such magnetic fields are achievable under laboratory conditions where inequality (1.1) is satisfied for fields of several Tesla, at $T \leq 1$ K. However, the gas of spin-polarised hydrogen atoms is thermodynamically unstable with respect to recombination, which gives rise to hydrogen molecules in the ground state Σ_g^+ showing enormously high binding energy (4.6 eV) compared with μB . For this reason, Bose condensation of spin-polarised hydrogen is possible only at sufficiently low density, and hence at very low temperature.

Of special interest under terrestrial conditions are excitons, for which the ultrahigh magnetic field condition (1.2) takes the form

$$B \gg B_{\rm ex} = \frac{m_{\rm eff}^2 e^3 c}{e^2 \hbar^3} \,. \tag{1.4}$$

In this situation, the strength of an ultrahigh magnetic field depends on the properties of the semiconductor. The magnetic field for excitons becomes already 'ultrahigh' if its strength is of the order of 1 T, owing to the small effective mass $m_{\rm eff}$ and large dielectric constant ε (particularly for direct-band semiconductors). For example, the field for Ge is strong at 9 kG or higher whereas the field for InSb may be considered strong starting from 2 kG. Modified properties of excitons in ultrahigh magnetic fields can be responsible for new, interesting physical phenomena. Owing to a marked rise of the exciton binding energy in a high magnetic field, the exciton fluid acquires the properties of a quasi-ideal Bose-gas which can give rise to Bose condensation, superfluidity of the exciton fluid, formation of exciton crystals, etc. Note that the formation of a Bose condensate of excitons in a high magnetic field is possible up to a density of the exciton liquid greater by a factor of $(B/B_{\rm ex}) \ln (B/B_{\rm ex})$ than the maximum density of excitons a_0^{-3} for which the Bose condensation is possible without a magnetic field. For higher exciton densities, when the overlap of the wave functions of excitons becomes noticeable, the ground state of the system will be an electron-hole liquid instead of the Bose condensate [101]. These effects are interesting not only for basic physics but also for the development of semiconductors with new unusual properties, such as supertransparency, superthermal conductivity, etc. [6, 7].

1.2 Pulsars — rotating magnetic neutron stars

Anyone dealing with physical aspects of magnetism would consider magnetic fields of 10^{12} to 10^{13} G utterly unrealistic, if not fantastic[†]. However, in 1967, a Cam-

†Maximal pulsed magnetic fields available in the laboratory can reach 25 MGs for explosive magnetic generators [1] and 40 MGs for pinch plasma linear compression of magnetic flux [9, 10].

bridge group of astronomers reported the discovery of pulsars, that is rotating magnetic neutron stars, having at their surface incredibly high magnetic fields of around $10^{12}-10^{13}$ G [11, 12]. Since then, studies of the properties of matter in such ultrahigh magnetic fields have exceeded the bounds of a purely academic problem.

The discovery of pulsars was a signal success of both astronomy and theoretical physics. The existence of neutron stars had been predicted long before the first pulsar was found [13, 14]. Interestingly, only a few months before Hewish and co-workers first reported their pulsar discovery in *Nature*, this journal had published a paper [15] in which the possibility of the generation of regular electromagnetic pulses by rapidly rotating magnetic neutron stars was introduced. In fact, pulsars appear to have been first invented by theoreticians and only afterwards proved to be existing entities.

Very soon after pulsars had been discovered, it was deduced, following a most trivial line of reasoning, that they were actually rapidly rotating magnetic neutron stars [16]. It was equally clear that such stars had to have extended atmosphere because of the enormously high electric field

$$E \approx \frac{1}{c} \Omega RB \approx 10^{12} \text{ V cm}^{-1} , \qquad (1.5)$$

near their surface, which is normally induced by the rotation of a highly magnetised neutron star with radius R and rotation frequency Ω . Actually, even if in the 'vacuum approximation' a pulsar generates magnetodipole emission (as it does in vacuum), all currently known pulsars may be expected to have ΩB values in the range 10^{12} to 10^{14} . In other words, the electric force that acts on a charged particle on the surface of a pulsar with pulsar mass close to that of the sun $(M_{\odot} = 1.99 \times 10^{33} \text{g})$ and radius $10^{-5}R_{\odot} \approx 10^{6} \text{ cm}$ ($R_{\odot} = 6.96 \times 10^{10} \text{ cm}$) is estimated as being seven or eight orders of magnitude higher than the gravitational force.

Huge magnetic fields of neutron stars (about $10^{11} - 10^{13}$ G) are formed in the course of their evolution. According to stellar evolution theory, a neutron star — i.e. the final phase of the evolution — is the product of a star with initial mass near the Chandrasekhar limit of $1.5M_{\odot} \leq M \leq 3M_{\odot}$ which has exhausted its thermonuclear energy and collapsed. Such stars are believed to be largely composed of iron atoms since it is known that a thermonuclear reaction becomes an endothermic reaction with elements heavier than ⁵⁶Fe [17].

A typical scenario for the formation of a neutron star normally implies the concurrent explosion of a supernova. The most 'famous' pulsar, PSR-0531 + 21, can be seen in the Crab nebula exactly where Chinese astronomers observed the bright explosion of a supernova in 1054. This pulsar has a rotation period of $P \approx 0.033$ s. Rotation periods of more than 1000 currently known pulsars are in the range 0.015 to 3.74 s [18].

Gravitational compression at the incredibly high densities in the centre of a star makes electron capture by protons as a result of the reaction $p + e^- \rightarrow v_e + n$ energetically favourable. The balance of pressure between the newly formed degenerate neutron fluid and the gravitational field accounts for the star reaching equilibrium and compression being terminated. The mass of a neutron star in equilibrium can be easily estimated by equating the pressure of the strongly degenerate neutron fluid with the density n in a star of radius R:

$$P_{\rm n} = \hbar c n^{4/3} \approx \frac{\hbar c N^{4/3}}{R^4}$$
 (1.6)

(where N is the total number of neutrons) with gravitational pressure

$$P_{\rm g} \approx G \, \frac{M^2}{R^4} \,, \tag{1.7}$$

where $G = 6.67 \times 10^{-8}$ dyn cm² g⁻² is the gravitational constant. In this case, the mass of the neutron star is

$$M_{\rm n} \approx \frac{1}{m_{\rm n}^2} \left(\frac{\hbar c}{G}\right)^{3/2} \approx 1.4 \, M_{\odot} \,, \qquad (1.8)$$

where m_n is the neutron mass and M_{\odot} is the mass of the sun. Density at the centre of the neutron star may be expressed as

$$\rho \approx \frac{m_{\rm n}}{(4\pi/3)(\hbar/m_{\rm n}c)^3} \approx 10^{16} \text{ g cm}^{-3} ,$$
(1.9)

whence the radius of the neutron star is

$$R_{\rm n} \approx \left(\frac{M_{\rm n}}{\rho}\right)^{1/3} \approx 10^{-5} R_{\odot} \approx 10^6 {\rm ~cm} \;.$$
 (1.10)

At high temperature and electric conductivity of the stellar matter, the initial magnetic field is compressed during collapse, frozen in the matter, and grows as

$$B_{\rm n} \propto B_0 \left(\frac{R_0}{R_{\rm n}}\right)^2 \,, \tag{1.11}$$

where (B_0, R_0) and (B_n, R_n) denote the initial and the final values of the magnetic field and radius, respectively. Hence, for typical stellar magnetic fields of about $10^2 - 10^3$ G, the magnetic field of a pulsar must be approximately $10^{12} - 10^{13}$ G, in agreement with the observed values.

It is worthwhile to note that the maximum value of the magnetic field for a neutron star can be estimated by means of the virial theorem and the assumption that a star of radius *R* has magnetic energy $(B^2/8\pi) \times 4\pi R^3/3$ identical to the gravitational energy GM^2/R . Hence, the maximum magnetic field of the neutron star may be described as

$$B_{\rm n,max} \sim 10^{18} \frac{M}{M_{\rm n}} \left(\frac{R}{R_{\rm n}}\right)^{-2} {\rm G} \; .$$

Interestingly, magnetic fields (unlike electric fields) have no upper limit on maximum value because of their conservatism. However, since the rotation of a neutron star induces electric field $E \approx c^{-1}\Omega RB$, the upper limit on this field implies that the maximum value of the parent magnetic field must likewise be limited. Hence, the highest magnetic field in pulsars presumably can hardly exceed $B \leq c E_{\text{max}}/\Omega R \sim 10^{15} \text{ G}.$

The surface temperature of newborn neutron stars is extremely high. However, the stars cool down very quickly owing to intense emission. For this reason, the surface temperature of even relatively young neutron stars must be around 100 eV. Older neutron stars (over one million years of age) are likely to have surface temperatures of 10-20 eV.

Huge magnetic fields ($B \sim 10^{12} \text{ G} \ge B_9$) are responsible for gross deformation of atoms in the thin surface layer of neutron stars, which results in complete restructuring of the 120

atomic shells and dramatic alteration of the interatomic interaction. Specifically, binding energy and ionisation potential of the atoms are greatly increased as compared with those observed under normal terrestrial conditions. This accounts for the high abundance of neutral atoms even at the fairly high temperatures at the surface of a neutron star. The properties of matter on the surface undergo equally pronounced changes. For instance, hydrogen atoms normally show strong interaction giving rise to molecules with binding energy of about 4.5 eV and they solidify forming a crystal at sufficiently low temperatures. However, interaction between these atoms becomes weaker following their complete polarisation in the magnetic field $B \gg B_9$. Moreover, totally polarised hydrogen atoms appear to acquire certain properties of helium. Gas of completely polarised hydrogen atoms in the ground state fails to solidify even at zero temperature. Indeed, it can form a Bose condensate and become superfluid at low temperatures.

Properties of matter and heavy atoms are also subject to marked alteration in ultrahigh magnetic fields. Atoms in the ground state exhibit weak interaction when polarised in a high magnetic field. This suggests that the surface layer of neutron stars should be composed either of fluid or of gas. The binding energy of the matter on the stellar surface is comparable with the surface temperature and is evidently smaller than the distance between the Landau levels $\mu B \sim \hbar \omega_{\rm c} \approx 11.7 \text{ keV}$ at $B = 10^{12} \text{ G}$. At the same time, excited atoms can be strongly interacting and assemble into molecules, long polymeric chains, and crystalline structures with binding energies considerably exceeding those of ordinary molecules and solids. It is worthwhile to note that the effects of magnetic fields on the properties of stellar matter are apparent only in the thin surface layer of neutron stars (about 1 m thick). Such effects are less conspicuous as the density of deeper layers grows and the mean distance between electrons $n_e^{-1/3}$ becomes smaller than their cyclotron radius at the lowest Landau level, that is at densities where the Fermi temperature $\hbar^2 n^{2/3}/m_e$ exceeds the magnetic energy μB . The corresponding density for the magnetic field $B \sim B_{12} \equiv 10^{12}$ G is about 10^6 g cm⁻³. It should be emphasised that the state of the stellar

It should be emphasised that the state of the stellar matter in ultrahigh magnetic fields at the surface of a neutron star surface remains to be elucidated. At the same time, the properties of the surface matter are crucial for both the theory of the pulsar magnetosphere and for understanding the nature of its emission. Moreover, this knowledge is indispensable for modelling the magnetosphere of pulsars. Indeed, rotation of a magnetised star produces an electric field with a component which is parallel to the magnetic field lines which can accelerate electric charges up to relativistic energies. These particles are thought to fill the pulsar magnetosphere and account for its electromagnetic radiation.

In early studies [19, 20] it was hypothesised that the strong interatomic interaction at the surface of a star may be responsible for the formation of matter with very high binding energy and work function (in excess of 3 keV) which can completely block the release of matter from the star. In such a case, a vacuum gap is likely to form near the surface in which a large part of the electric potential $\Delta \varphi \sim 10^{12}$ V is developed. Breakdown in the gap results from the cascade process of formation of electron – positron pairs [21] or from their production by γ -quanta [22, 23]. The theory of the pulsar magnetosphere for the case of

stellar matter completely trapped in the surface layer has been examined at greater length in monograph [24].

During the last 10 years, different authors [25-29] have demonstrated that in the case of atoms completely polarised in a strong magnetic field, interatomic interactions are much weaker, and hence binding energy and work function are lower (always below 1 keV), than they were believed to be in earlier studies. Therefore, models assuming large work function and complete trapping of charged particles appear to be lacking in self-consistency [30-32].

If the work function is small, a 'free-emission' model of the pulsar is applicable which implies that the domains where the magnetic lines are closed are filled with plasma whereas in the domains with open magnetic lines, release of particles is very near to the limit associated with the entire screening of the electric field in this domain [33, 34]. It cannot be ruled out that other processes, e.g. electrohydrodynamic instability [35], also affect the structure of the pulsar magnetosphere.

It may be concluded that structural features of the magnetosphere largely depend on the scenario of charge outflow, which actually occurs. Therefore, understanding the physical properties of the surface matter in a strong magnetic field is of paramount importance for pulsar physics.

According to stellar evolution theory, the surface of a neutron star is composed of heavy elements, in the first place of iron atoms. However, neutron stars are believed eventually to contain light atoms as well (especially those of helium) owing to their accretion from the interstellar space or from a companion star (in the case of binary stars) [36, 37]. This process should be accompanied by sinking of heavy atoms, with light ones remaining at the surface. Therefore, 'old' neutron stars can be expected to have both their atmosphere and their surface grossly enriched with hydrogen and helium at relatively low surface temperatures (10 eV) whereas the surface of 'younger' stars must be largely composed of iron at the surface temperature of about 100 eV. Thus, the properties of matter in a strong magnetic field are of great interest whether it consists of light atoms or heavy ones.

It is equally conceivable that an intermediate scenario applies as regards certain pulsars, in compliance with the model of the magnetosphere with free emission at the beginning of the pulsar's life or the model with trapped emission for older pulsars if the binding energy of the lattice of alternate heavy and light atoms is sufficiently high.

2. Hydrogen atom in an ultrahigh magnetic field

The problem of the hydrogen atom in ultrahigh magnetic fields was first examined in connection with the behaviour of hydrogen-like excitons (the so-called Vanie-Mott excitons) in semiconductors placed in a strong magnetic field [38-40]. It the case of hydrogen-like excitons in a semiconductor the 'ultrahigh' magnetic field is actually not very high because of the small effective mass of the electron and high dielectric permeability of the semiconductor. For excitons in InSb, for example, a magnetic field of 2 kG is readily available in the laboratory, corresponding to a magnetic field $B_9 = 2.35 \times 10^9$ G for a hydrogen atom.

The nonseparability of the Schrodinger equation for an electron in a combined uniform magnetic field and the Coulomb field makes it impossible to obtain an exact solution even for such a simple problem as the hydrogen atom in a uniform magnetic field. This problem has been a challenge to novel methods of perturbation theory as well as other methods, including the variational approach, the adiabatic approximation, etc. This is by no means the case for the quadratic Zeeman effect, and the problem becomes quite difficult when the two field strengths are comparable. There are difficulties with the classification of the energy terms even for a weak magnetic field (linear Zeeman effect)-despite numerous investigations (including perturbation, semiclassical and quantum calculations, and numerical calculations), it is not yet possible to predict even quantitatively the evolution of arbitrary energy levels as a function of magnetic field strength from the zero-field limit for the regime where the magnetic field is comparable with Coulomb fields. So far, the quadratic Zeeman effect and the general problem of a hydrogen atom in a magnetic field labelled as 'trouble with hydrogen' remain one of the major unsolved basic problems of atomic physics. The intrinsic theoretical interest of such a problem together with its obvious applications to atomic spectroscopy, astrophysics, and the physics of semiconductors have generated a great deal of interest in the subject. A good general review of the Zeeman effect up to 1977 has been given by Garstang [53], while more specialised articles have appeared in Refs [49-56].

For the limiting case of a very high magnetic field the solution of the problem can be easily obtained with logarithmic accuracy (see also Ref. [41], p. 112 and problems 1-3). The distance between Landau levels $\hbar\omega_c$ in ultrahigh magnetic field $B \ge B_9$ is much greater than the energy of Coulomb interaction, which is equivalent to the condition

$$\frac{e^2}{a_0} \ll \hbar \omega_{\rm c} , \qquad (2.1)$$

where $a_0 \equiv \hbar^2/m_e e^2$ is the Bohr radius. This condition implies that the electron is at the lowest Landau level while the atom undergoes deformation and turns into a thin tubule with radius $\rho_0 = (\hbar c/eB)^{1/2} \ll a_0$ and length $L < a_0$ oriented parallel to the magnetic field lines.

The energy of the hydrogen atom's ground state can be estimated from a simple model. Assume that the energy of the ground state consists of the kinetic energy of motion along the magnetic field lines (axis z) with momentum $p_z \approx \hbar/L$, and the potential energy of a uniformly charged tubule of radius ρ_0 and length L:

$$\mathcal{E} \approx \frac{\hbar^2}{2m_{\rm e}L^2} - \frac{e^2}{L} \ln \frac{L}{\rho_0} \,. \tag{2.2}$$

By minimising \mathcal{E} , it is possible to obtain from Eqn (2.2), with logarithmic accuracy,

$$L \approx a_0 \ln^{-1} \frac{a_0}{\rho_0}$$
, (2.3)

$$\mathcal{E} \approx -\frac{\hbar^2}{2m_{\rm e}a_0^2}\ln^2\frac{a_0}{\rho_0}\,.\tag{2.4}$$

Formally, a more strict solution is available by use of the so-called adiabatic approximation. Consider the Coulomb interaction between the electron and the nucleus to be a small perturbation of the electron motion in a homogeneous magnetic field. The Schrodinger equation for the hydrogen atom in a magnetic field has the form

$$\left[\frac{1}{2}\left(-i\hat{\nabla}+A\right)^{2}-\frac{1}{r}+\frac{1}{2}\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{B}\right]\boldsymbol{\Psi}=E\boldsymbol{\Psi}.$$
(2.5)

Here, it is convenient to use atomic units $e = m_e = \hbar = c = 1$ and express the magnetic field in units of $B_9 = 2.35 \times 10^9$ G. Let the axis z be along the direction of the magnetic field lines and choose the usual gauge for the vector potential $A = (B \times r)/2$. In the first order in $1/B \leq 1$, the electron wave function can be presented as

$$\Psi(\mathbf{r}) = \psi_{n_o,m}(\rho, \varphi) f_{\nu}(z) , \qquad (2.6)$$

where

ψ

$${}_{n_{\rho},m}(\rho,\varphi) = \frac{\exp(\mathrm{i}m\varphi)}{\sqrt{2\pi}} \rho_{0}^{-1-|m|} \left[\frac{(|m|+n_{\rho})!}{2^{|m|}n_{\rho}!|m|!} \right]^{1/2} \times \rho^{|m|} \exp\left(-\frac{\rho^{2}}{4\rho_{0}^{2}}\right) P_{n_{\rho},m}\left(\frac{\rho^{2}}{2\rho_{0}^{2}}\right)$$
(2.7)

is the wave function of free transverse motion of the electron in the magnetic field [41] and $f_v(z)$ is the solution of the Schrodinger equation obtained by averaging Eqn (2.5) over functions $\psi_{n_p,m}(\rho,\varphi)$. Here, $\rho = \sqrt{x^2 + y^2}$ is the polar coordinate in the x-y plane, φ is the angular coordinate, and $P_{n,m}(x)$ are the Laguerre polynomials. Note that the radius of the lowest Landau orbit in atomic units is $\rho_0 = 1/\sqrt{B}$.

The lowest Landau level at $n_{\rho} = m = 0$ corresponds to the minimum energy state. The corresponding equation for $f_{\nu}(z)$ has the form

$$\left[-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}z^2} + U(z)\right]f_{\nu} = \mathcal{E}f_{\nu} , \qquad (2.8)$$

where the binding energy is

$$\mathcal{E}=\frac{1}{2} B-E ,$$

and the potential is

$$U(z) = -\frac{1}{\rho_0^2} \int \frac{\rho \, d\rho}{\sqrt{\rho^2 + z^2}} \exp\left(-\frac{\rho^2}{2\rho_0^2}\right) \,. \tag{2.9}$$

For the approximate solution of Eqn (2.8), potential (2.9) may be approximated by the expression [42]

$$U(z) \approx -\frac{1}{a+|z|} + \frac{A}{(a+|z|)^2},$$
 (2.10)

where the parameters a and A depend on the magnetic field and the quantum numbers n_{ρ} and m. The problem can be reduced to the one-dimensional Shrodinger equation with potential U(z) turning to the 1d-Coulomb potential at distances which may be considered great compared with the 'size' of the atom, i.e. at $z \approx 1 \ge 1/\sqrt{B}$. The solution of Eqn (2.8) with the potential (2.10) which describes ground state $f(z) \equiv f_{\nu=0}(z)$ can be expressed through the Whittaker functions:

$$f(z) = \frac{1}{\sqrt{\alpha}} W_{\alpha, 1/2} \left[\frac{2}{\alpha} (z + \rho_0) \right], \qquad (2.11)$$

where symbol α in Eqn (2.11) is analogous to the principal quantum number in the hydrogen atom problem, i.e.

$$\mathcal{E} \sim -\frac{1}{2\alpha^2} \,. \tag{2.12}$$

It is possible to derive an asymptotic expression for the ground state energy. For $\ln B \ge 1$, with logarithmic accuracy $\alpha \approx 1/\ln B$, Eqn (2.12) implies expression (2.4) for the ground state energy:

$$\mathcal{E} \sim -\frac{1}{2} \ln^2 B \ . \tag{2.13}$$

It should be noted that the solution of the problem for the binding energy of hydrogen in a strong magnetic field is asymptotic and can be obtained only with logarithmic accuracy. Formula (2.13) provides only the main term of the expansion; not only is $B \to \infty$ required but also $\ln B \to \infty$. Therefore, for magnetic fields $B = 10^{12}$ G, intrinsic in neutron stars, expression (2.13) gives correct values of the ground state energy only up to the order of magnitude. Many authors used different approximate approaches that allowed hydrogen energy (at $B \ge 1$) to be estimated with accuracy acceptable for the comparison with the observed values [39, 43-46]. However, it appears impossible to obtain better than 20% accuracy of the approximate formulas if calculation methods are in one way or other based on the approximate problem of onedimensional motion in a modified Coulomb field.

Since the problem is of great interest in astrophysics, the spectrum of a hydrogen atom in a strong magnetic field has been calculated [47–51] (see also the review of approximate and numeric methods in Ref. [52]). Fig. 1 shows the ground state binding energy of hydrogen atoms as a function of the magnetic field strength for the lowest Landau level $n_{\rho} = 0$, m = 0, and for the projections of orbital momentum m = 1, 2, 3. For the magnetic field $B = 10^{12}$ G characteristic of neutron stars, the hydrogen ionisation potential is about 160 eV.

In the ground state, electron spin is tightly fixed and directed against the field. The energy needed for spin flip is unusually high. Specifically, it amounts to $\mu B \approx 11.6$ keV for



Figure 1. Binding energy, \mathcal{E} , of the ground state (m = 0) and the first excited states of a hydrogen atom for m = 1, 2, 3, as a function of the magnetic field strength, B.

the magnetic field $B = 10^{12}$ G. Excited states in the discrete spectrum arise as solutions of the Shrodinger equation (2.8) in the one-dimensional Coulomb field and corre-spond to the wave functions having zeros at finite z. (The ground state wave functions have no zeros in z). The spectrum of the excited states of hydrogen in a strong magnetic field is in a way reminiscent of that of the hydrogen atom without a magnetic field. $\mathcal{E}_n \approx -1/2n^2$ is the expression for energy levels with logarithmic accuracy. These excited states are close to the top of the discrete spectrum, and their binding energy does not significantly differ from that of a normal hydrogen atom (13.6 eV). Complete solution of the problem of the hydrogen spectrum in an arbitrary magnetic field requires rather cumbersome computation [50, 51, 53-56].

The complete set of quantum numbers for hydrogen in a strong magnetic field consists of spin projection s_z , Landau level number n_p , the number of nodes v of the wave function $f_v(z)$, and projection of orbital momentum m. The first two quantum numbers in the ground state at $B \ge 1$ are fixed. At $B \ge 1$, the spin projection $s_z = -1/2$, which makes it possible to restrict examination to the lowest Landau level $n_p = 0$. In this case, the radial part of the wave function together with the usual dependence on azimuthal angle is:

$$\psi_{n_{\rho},m}(\rho, \varphi) = \frac{\exp(im\varphi)}{\sqrt{2\pi}} \frac{1}{\sqrt{2^{|m|}}} \frac{1}{\rho_0} \left(\frac{\rho}{\rho_0}\right)^{|m|} \exp\left(-\frac{\rho^2}{4\rho_0^2}\right).$$
(2.14)

Unlike energy for free electron motion, which is independent of the angular moment projection, the ground state energy shows weak dependence on m [19, 57, 58,], and the discrete spectrum contains excitations corresponding to different values of cyclotron radius $\rho_m = \sqrt{2m + 1}\rho_0$. Respective energy values can be obtained from Eqn (2.4) after the substitution $\rho_0 \rightarrow \rho_m$ so that

$$\mathcal{E}_{n_{\rho}=0,m} \approx -\frac{1}{2} \ln^2 \frac{B}{\sqrt{2m+1}}$$
 (2.15)

Note once again that analytical expressions for the energy are in fact asymptotic formulas derived with logarithmic accuracy, i.e. with $\ln B \ge 1$ at least. For this reason, they give correct values of binding energy only to within an order of magnitude. It follows from Eqn (2.15) that the distance between levels *m* and *m* + 1 for *m* ≥ 1 is approximately

$$\Delta \mathcal{E}_{m,m+1} \approx \frac{1}{2m+1} \ln \frac{B}{\sqrt{2m+1}} \ll \ln^2 B . \qquad (2.16)$$

Note also that the problem for a hydrogen-like atom with nuclear charge Z may actually be reduced to that of the hydrogen atom, taking into account that [57, 59]

$$E(Z, B) = Z^2 E\left(1, \frac{B}{Z^2}\right)$$

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3. Hydrogen molecule in an ultrahigh magnetic field

Interatomic interaction in an ultrahigh magnetic field and the formation of molecules and bound states is one of the most intriguing problems in pulsar physics. Its simplest version is the problem of the hydrogen molecule in an ultrahigh magnetic field.

It should be borne in mind that two hydrogen atoms in the ground state give rise to a system with two molecular terms: singlet ${}^{1}\Sigma$ and triplet ${}^{3}\Sigma$ [41]. A major contribution to the interatomic interaction at large distances is provided by the van der Waals forces, whereas the exchange interaction plays a key role at smaller distances comparable with the atom's size. The ground term is ${}^{1}\Sigma$ while the term ${}^{3}\Sigma$ has a higher energy since the coordinate part of the wave function of two electrons for ${}^{3}\Sigma$ is antisymmetric, in conformity with the Pauli principle, and becomes zero in the symmetry plane of the molecule. In other words, the antisymmetric wave function corresponds to the electron density distribution (with electrons being located near their nuclei) and to the effective repulsion of atoms which accounts for the monotonic growth of the interatomic interaction potential for term ${}^{3}\Sigma$ as the atoms draw together. On the other hand, overlapping of wave functions for term ${}^{1}\Sigma$ results in a deep potential well which leads to the formation of hydrogen molecules at the internuclear distance of the order of a_0 and the binding energy of around 4.5 eV.

The situation dramatically changes in the presence of an ultrahigh magnetic field where atoms, grossly deformed and elongated parallel to the magnetic field lines, interact at large distances as quadrupoles. The most significant difference is that the ground state in this situation is term ${}^{3}\Sigma$, since atoms in this state have negative additional energy of the order of $\mu B \gg Ry$.

Interatomic interaction in both singlet and triplet terms of the hydrogen molecule placed in an ultrahigh magnetic field can be calculated with logarithmic accuracy [60, 61]. The Shrodinger equation for two hydrogen atoms (in atomic units) has the form:

$$\begin{bmatrix} \frac{1}{2} (\hat{P}_1 + \hat{A}_1)^2 + \frac{1}{2} (\hat{P}_2 + \hat{A}_2)^2 - \sum_i \frac{1}{R_{1i}} - \sum_i \frac{1}{R_{2i}} \\ + \frac{1}{r_{12}} + \frac{1}{R} + \frac{1}{2} \hat{\sigma}_1 \cdot \mathbf{B} + \frac{1}{2} \hat{\sigma}_2 \cdot \mathbf{B} \end{bmatrix} \Psi = E \Psi .$$
(3.1)

where R is the distance between atomic nuclei 1 and 2, R_{1i} and R_{2i} are distances between the *i*th electron and nuclei 1 and 2 respectively, and r_{12} is the distance between electrons. By choosing the gauge for the vector potential $A = (\mathbf{B} \times \mathbf{r})/2$, one can present Eqn (3.1) as

$$\left[\mathcal{H}(1, 2) + \frac{1}{2}\hat{\boldsymbol{\sigma}}_{1} \cdot \boldsymbol{B} + \frac{1}{2}\hat{\boldsymbol{\sigma}}_{2} \cdot \boldsymbol{B}\right]\boldsymbol{\Psi} = \boldsymbol{E}\boldsymbol{\Psi}, \qquad (3.2)$$

where

$$\mathcal{H}(1, 2) = -\frac{1}{2} \nabla_{1}^{2} - \frac{1}{2} \nabla_{2}^{2} - \frac{1}{2} \mathbf{B} \cdot (\mathbf{r}_{1} \times \nabla_{1}) - \frac{1}{2} \mathbf{B} \cdot (\mathbf{r}_{2} \times \nabla_{2})$$
$$-\sum_{i} \frac{1}{R_{1i}} - \sum_{i} \frac{1}{R_{2i}} + \frac{1}{R} + \frac{\rho_{1}^{2} + \rho_{2}^{2}}{8\rho_{0}^{4}}.$$
 (3.3)

Here, axis z is directed along the magnetic field lines, and atoms in the x-y plane have coordinates

$$x_{1,2} = \mp a = \mp \frac{R}{2} \cos \theta$$
, $z_{1,2} = \mp b = \mp \frac{R}{2} \sin \theta$, (3.4)

where θ is the angle between the molecule axis and the direction of the magnetic field lines, while $\rho_1^2 = y_1^2 + (b + x_1)^2$ and $\rho_2^2 = y_2^2 + (b - x_2)^2$ are the polar coordinates of electrons 1 and 2, respectively, in the x - y plane.

Denoting the symmetric (s) and antisymmetric (a) coordinate parts of the wave function for the singlet and

the triplet terms by Ψ_s and Ψ_a respectively, also taking into account that for ${}^{1}\Sigma$ the total spin S = 0 and the ground state for ${}^{3}\Sigma$ in an ultrahigh magnetic field corresponds to the total spin projection S = -1, one can write equations for Ψ_s and Ψ_a as

$$\mathcal{H}(1,\,2)\Psi_{\rm s} = E_{\rm s}\Psi_{\rm s} \,\,, \tag{3.5}$$

$$\left[\mathcal{H}(1, 2) - \frac{1}{\rho_0^2}\right] \Psi_{\rm a} = E_{\rm a} \Psi_{\rm a} .$$
(3.6)

It is convenient to rewrite these equations for Ψ_s and Ψ_a as a single equation introducing $E_{s1} = E_s - 1/\rho_0^2$. Then,

$$\left[\mathcal{H}(1, 2) - \frac{1}{\rho_0^2}\right] \Psi_{s,a} = E_{s1,a} \Psi_{s,a} .$$
(3.7)

Using the approach described in [62, 63], one can obtain asymptotically accurate expressions for the difference between energies of singlet and triplet terms owing to the exchange interaction. To this end, it is necessary to examine the functions $\Psi_1 = (\Psi_s + \Psi_a)/2$ and $\Psi_2 = (\Psi_s - \Psi_a)/2$ corresponding to the respective states in which each electron at large *R* is located near its own nucleus.

Functions Ψ_1 and Ψ_2 can be found in the form of the product of wave functions for two hydrogen atoms:

$$\Psi_{1} = \frac{1}{2\pi\alpha\rho_{0}^{2}}\chi_{1}\exp\left(-\frac{\rho_{1}^{2}+\rho_{2}^{2}}{4\rho_{0}^{2}}\right)$$
$$\times W_{\alpha,1/2}\left[\frac{2}{\alpha}(a+z_{1}+\rho_{0})\right]W_{\alpha,1/2}\left[\frac{2}{\alpha}(a-z_{1}+\rho_{0})\right], (3.8)$$

where χ_1 is a function changing slowly compared with the exponent in Eqn (3.8). The equation for χ_1 with accuracy up to terms of the first order of magnitude in $\alpha \ll 1$ has the form

$$\left(\frac{1}{\alpha}\frac{\partial}{\partial z_1} - \frac{1}{\alpha}\frac{\partial}{\partial z_2} - \frac{2}{R_{12}} + \frac{1}{r_{12}} + \frac{1}{R}\right)\chi_1 = 0.$$
(3.9)

(A similar equation for χ_2 is obtainable with the substitution $1 \leftrightarrow 2$.)

Energy splitting in singlet and triplet terms is expressed through the integral of the product $\Psi_1\Psi_2$ over the hypersurface $S(z_1 = z_2)$ in the space $\{r_1, r_2\}$ [62, 63]:

$$E_{s1} - E_{a} = 2 \oint_{S(z_{1}=z_{2})} (\Psi_{2} \nabla_{1} \Psi_{1} - \Psi_{1} \nabla_{1} \Psi_{2}) \,\mathrm{d}s \;. \tag{3.10}$$

Based on the solutions of Eqn (3.9) [60] and calculating the integral in Eqn (3.10), the following expression can be found for the exchange part of the term splitting energy:

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$$\Delta E = (E_s - B) - E_a$$

$$= -\frac{2R\ln^2 B}{\cos^2 \theta} \left(2\cos\theta \ln B + \frac{1}{2}RB\sin^2\theta \right)$$

$$\times \exp\left[-R\left(2\cos\theta \ln B + \frac{1}{4}RB\sin^2\theta \right) \right] . (3.11)$$

At distances exceeding the atomic size along the magnetic field lines $(r \ge 1/\ln B)$, the interatomic interaction is of the quadrupole-quadrupole type. Bearing in mind that quadrupole momentum of the atom at $\alpha \approx 1/\ln B \ll 1$ is $Q = 2\langle z^2 \rangle \approx \alpha^2/2$, the equation for the

potential of quadrupole-quadrupole interaction has the form

$$U_{qq} = \frac{9}{8} \frac{1}{\ln^4 B} \frac{1}{R^5} P_4(\cos\theta) , \qquad (3.12)$$

where

$$P_4(\cos\theta) = \frac{1}{8}(35\cos^4\theta - 30\cos^2\theta + 1)$$

is the 4th-degree Legendre polynomial.

Formulas (3.11) and (3.12) give expressions for the potentials of the interaction between two hydrogen atoms in the ground state in an ultrahigh magnetic field for singlet and triplet terms:

$$U_{\rm S} = -\frac{1}{2}\,\Delta E + B + U_{\rm qq} \,\,, \tag{3.13}$$

$$U_{\rm T} = \frac{1}{2} \,\Delta E + U_{\rm qq} \,\,. \tag{3.14}$$

The negative energy minimum for the quadrupolequadrupole interaction is reached at $\theta \approx 49^{\circ}$. Note that the exchange energy of term splitting at $r \to \infty$, minus the energy difference $\Delta U = B$, becomes exponentially small compared with the power fall-off of the quadrupolequadrupole interaction. Therefore, the difference between energies $U_{\rm S}$ and $U_{\rm T}$ is on the whole determined by the magnetic field $B \ge 1$ whereas the depth of the potential well $U_{\rm S}$ and $U_{\rm T}$ at $R \le 1$ is largely dependent on the exchange interaction.



Figure 2. Potential of hydrogen interactomic interaction in (a) singlet and (b) triplet terms in a magnetic field $B = 100 B_9 = 2.35 \times 10^{11} \text{ G}$.



Figure 3. (a) The sizes of the potential well, and (b) the depth of the potential well for the singlet (R_S, U_S) and for the triplet (R_T, U_T) terms of a hydrogen molecule as functions of the strength of the magnetic field (*B* is in units of $B_9 = 2.35 \times 10^9$ G).

The interaction potential of two hydrogen atoms in a strong magnetic field ($B = 100 B_9 = 2.35 \times 10^{11} \text{ G}$) for singlet and triplet terms are shown in Fig. 2. In the ground state corresponding to the triplet term, the interaction between hydrogen atoms is very weak, with the depth of the potential well being smaller than 0.1 eV. At the same time, the well depth in the singlet term is about 500 eV. However, the energy difference between the singlet and triplet terms at $B = 100 B_9$ is $\Delta E \approx \mu B \approx 2.7$ keV.

The depth of the potential well for both singlet and triplet terms increases with increasing magnetic field, whereas positions of minima (molecular size), $R_{\rm S}$ and $R_{\rm T}$, decrease. In strong magnetic fields where the molecular size approaches that of atoms ($B \ge 1000 B_9$), the difference between the singlet and the triplet states appears to be insignificant; instead, the formation of molecules becomes energetically favourable (Fig. 3).

For intermediate magnetic fields, singlet and triplet terms in the ground states of hydrogen molecules have been examined numerically at an arbitrary field orientation relative to the molecular axis [64]. The results of numerical calculations are in good agreement with analytic solutions of Eqns (3.13) and (3.14).

4. Bose-condensation and superfluidity of hydrogen in a strong magnetic field

Terms of a hydrogen molecule yield the potential of the pair interatomic interaction, which is sufficient for the description of a low-density gas, i.e. at $R_0 n^{1/3} \ll 1$, where R_0 is the characteristic scale of interatomic interaction (position of minimum in the pair interaction potential) and n is the gas density. Since the atomic size decreases with a rise in the magnetic field strength, the 'diluted' gas condition in an ultrahigh magnetic field is true even for relatively high densities. That is, the condition $R_0 n^{1/3} \ll 1$ is met for $B = 10^{12}$ G up to $n \leqslant 10^{29}$ cm⁻³.

The shallowness of the potential well in the ground state of the triplet term, and hence in the weak interatomic interaction, is associated with a conspicuous change in the properties of hydrogen gas in an ultrahigh magnetic field. Specifically, the interatomic interaction is so weak that hydrogen, similar to helium, fails to be frozen even at absolute zero. Also, it forms a Bose condensate and undergoes phase transition to the superfluid state at sufficiently low temperatures $T \leq \hbar^2 n^{2/3}/M$ [65]. Indeed, the energy of zero oscillations of the hydrogen atom is $\hbar^2 n^{2/3}/M \approx 0.5-5 \text{ eV}$, at a density of $n = 10^{27} - 10^{28} \text{ cm}^{-3}$, where M is the atomic mass. The energy of interatomic interaction in the ground state is comparable with the depth of the potential well in the triplet term $U_0 \equiv 10^{-2} - 10^{-1} \text{ eV}$ at $B = 10^{11} - 10^{12} \text{ G}$, whereas electron binding energy in the atom is of the order of 100 eV or higher.

The pair-interaction potential between hydrogen atoms in a strong magnetic field can be represented as

$$U(R, \theta) = \frac{1}{R} \exp\left(-\frac{R^2}{2R_0^2}\right) + U_0 \exp\frac{R}{R_0} P_4(\cos\theta) , \quad (4.1)$$

where R is the distance between the centres of mass of two atoms and the atomic nucleus, while U_0 and R_0 are the depth and the effective size of the potential well, respectively, which depend on the magnetic field strength and may be approximately written in the form

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$$R_0 \approx \frac{7.9}{\sqrt{B}},$$

$$|U_0| \approx 2.33 \ln^2 B \left(10.34 \frac{\ln B}{\sqrt{B}} + 41.6 \right)$$

$$\times \exp\left(-10.34 \frac{\ln B}{\sqrt{B}} - 8.92\right) - 3.66 \times 10^{-5} \frac{B^{5/2}}{\ln^4 B}$$

The hydrogen atom gas is supposed to be a weakly nonideal Bose gas of structureless particles because of the high binding energy of the electrons in hydrogen atoms and weak interatomic interaction. At temperatures lower than the temperature of transition to the Bose condensate, the

†A possibility of hydrogen being superfluid on the neutron star's surface scarcely affects its properties or those of the pulsar magnetosphere. Of greater importance is the low energy of interatomic bonds. The behaviour of excitons in a semiconductor placed in a strong magnetic field is responsible for quite a different situation because the small mass and high dielectric permeability of excitons allow for their Bose condensation and superfluidity at the magnetic field values of several Teslas attainable under laboratory conditions and even at room temperature [6, 7]. properties of such a gas are defined by normal and anomalous Green functions:

$$G_{N}(p) = \left[i\omega + \frac{k^{2}}{2m} - \mu + A(-p)\right] \\ \times \left\{\left[i\omega + \frac{k^{2}}{2m} - \mu + A(-p)\right] \\ \times \left[i\omega - \frac{k^{2}}{2m} + \mu - A(p)\right] + |B(p)|^{2}\right\}^{-1}, \quad (4.2)$$
$$G_{A}(p) = -B(p)\left\{\left[i\omega + \frac{k^{2}}{2m} - \mu + A(-p)\right] \\ \times \left[i\omega - \frac{k^{2}}{2m} + \mu - A(p)\right] + |B(p)|^{2}\right\}^{-1}, \quad (4.3)$$

where $p = (\mathbf{k}, \omega)$, $\omega \equiv \omega_s = 2\pi sT$ (s being an integer), μ is the chemical potential, and A(p) and B(p) are the irreducible self-energy functions [68].

The summation of diagrams making major contribution to the self-energy functions A(p) and B(p) can be expressed through the scattering amplitude in the momentum representation:

$$\frac{4\pi}{m}f(\mathbf{k}, \mathbf{k}') = U(\mathbf{k} - \mathbf{k}') + \sum_{n=1}^{\infty} \frac{1}{(2\pi)^{3n}} \int d\mathbf{k}_1 \dots d\mathbf{k}_n$$
$$\times \frac{U(\mathbf{k}' - \mathbf{k}_1) \dots U(\mathbf{k}_n - \mathbf{k})}{[(k^2 - k_1^2)/m + \mathrm{i}\delta] \dots [(k^2 - k_n^2)/m + \mathrm{i}\delta]}, \quad (4.4)$$

where $U(\mathbf{k} - \mathbf{k}')$ is the Fourier representation of the potential (4.1).

In calculating (4.4), a major contribution comes from the integration region with $k \ge 1/R_0$, i.e. the isotropic part of the potential in the momentum representation $U(\mathbf{k} - \mathbf{k}') \approx V_0$. Therefore, it follows from (4.4) with accuracy to the small terms of the order of $\rho_0/R_0 \ll 1$ that

$$\frac{4\pi}{m}f(\boldsymbol{k},\boldsymbol{k}')\approx V_0+U_{\rm A}(\boldsymbol{k}-\boldsymbol{k}') , \qquad (4.5)$$

where V_0 and U_A are the isotropic and anisotropic parts of $U(\mathbf{k} - \mathbf{k}')$, respectively. It is possible to demonstrate [65] that in the Born approximation (at $k \ll 1/\rho_0$)

$$V_0 \approx 4\pi \rho_0^2 = \frac{4\pi}{B} = \text{const}$$
 (4.6)

Taking into account (4.1) for the anisotropic part of the potential we obtain

$$U_{\rm A}(\boldsymbol{k}) = U_0 \int \exp\left[-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R} - \frac{R}{R_0}\right] P_4(\cos\,\theta)\,\mathrm{d}^3r\,,\qquad(4.7)$$

from which

$$U_{\rm A}(\boldsymbol{k}) = 4\pi U_0 R_0^7 k^4 J(kR_0) P_4(\cos\theta) , \qquad (4.8)$$

is derived by simple calculation, where the function $J(kR_0)$ is expressed through the 4th-order spherical Bessel functions j_4 :

$$J(kR_0) = \frac{1}{(kR_0)^4} \int_0^\infty j_4(kR_0x) e^{-x} x^2 dx .$$
 (4.9)

If the total atomic density is denoted by n, particle density in the condensate by n_0 , and noncondensed particle density by n_p , expressions for the self-energy functions can

be given through the momentum representation of the scattering amplitude:

$$A(\mathbf{k}) \approx n[2V_0 + U_A(\mathbf{k})], \qquad (4.10)$$

$$B(\boldsymbol{k}) \approx n[V_0 + U_A(\boldsymbol{k})] . \tag{4.11}$$

Using the Hugenholtz-Pains relation for chemical potential $\mu = A(0) - B(0)$, one can write the equation for the particle density in the condensate as

$$n_0 = \frac{\mu}{V_0} - 2n_{\rm p} \ . \tag{4.12}$$

The density of noncondensed particles can be presented in the form

$$n_{\rm p} = -\frac{T}{V} \sum_{p,\epsilon \to 0} \exp(\mathrm{i}\omega\epsilon) \, G^0(p) = \frac{\zeta(3/2)}{(2\pi)^{3/2}} \, (mT)^{3/2} \, , \quad (4.13)$$

where $\zeta(x)$ is the Riemann zeta function, $\zeta(3/2) = 2.612$, and

$$G^{0}(p) = \frac{1}{i\omega - k^{2}/2m + \mu}$$
(4.14)

is the unexcited Green function.

There is only one normal Green function, G(p), above the Bose condensation critical temperature. Since $n_0 = 0$ at a temperature higher than critical, it follows that

$$G(p) = \frac{1}{i\omega - (k^2/2m - \mu) - A(k)},$$
(4.15)

where A(k) is defined by Eqn (4.10).

The excitation spectrum of the system is determined by the poles of the Green function. Therefore, taking into account relations (4.10) and (4.11) for A(k) and B(k), we have

$$E(k) = \left[\left(\frac{k^2}{2m} - \mu \right)^2 + 2 \left(\frac{k^2}{2m} - \mu \right) A(k) + A^2(k) - B^2(k) \right]^{1/2} .$$
 (4.16)

The use of the expression for the chemical potential and the explicit form of A(k) and B(k) gives

$$E(k) = \left\{ \left[\frac{k^2}{2m} + n \times 4\pi U_0 R_0^7 k^4 J_0(kR_0) P_4(\cos\theta) + n_0 V_0 \right]^2 - \left[n \times 4\pi U_0 R_0^7 k^4 J_0(kR_0) P_4(\cos\theta) + n_0 V_0 \right]^2 \right\}^{1/2}.$$
 (4.17)

Expression (4.17) for E(k) is actually the Bogolyubov excitation spectrum, which fulfils the Landau criterion for superfluidity. It can be shown that in spite of the fact that the energy spectrum has a strong angular dependence on the direction of the magnetic field, the velocity of sound does not depend on the direction of the magnetic field to the first approximation, and the phonon branch at $k \rightarrow 0$ satisfies the Landau criterion for superfluidity:

$$E(k \to 0) \approx k \sqrt{\frac{4\pi n_0}{mB}} . \tag{4.18}$$

Therefore, the speed of sound in the superfluid phase is

$$u_{\rm s} \approx \sqrt{\frac{4\pi n_0}{mB}} \,. \tag{4.19}$$

The temperature of transition to the Bose condensate is found from the condition that particle density beyond the condensate, n_p , in the transition point (at $T = T_c$) must be equal to the total particle density n. Density n_p is expressed through the normal Green function. Above the transition temperature we have

$$n_{\rm p} = -\frac{T}{V} \sum_{p,\varepsilon \to 0} \exp(\mathrm{i}\omega\varepsilon) G(p)$$
$$= \frac{1}{(2\pi)^3} \int \frac{\mathrm{d}^3 k}{\exp[E(k)/T] - 1} \,. \tag{4.20}$$

Substitution of the expression for E(k) into Eqn (4.20) yields

$$n_{\rm p} = \frac{\zeta(3/2)}{(2\pi)^{3/2}} (mT)^{3/2} + \frac{\sqrt{2}}{\pi^2} m^{3/2}T$$
$$\times \left[\frac{\sqrt{\epsilon_2}}{2} \ln \frac{1 + \sqrt{\epsilon_1/\epsilon_2}}{1 - \sqrt{\epsilon_1/\epsilon_2}} - \sqrt{\epsilon_1 - n_0 V_0}\right], \qquad (4.21)$$

Assuming that in Eqn (4.21), $n_p = n$, $n_0 = 0$, it is possible to obtain the equation for the critical temperature of transition to the superfluid state. The $T_c(n)$ dependence for three magnetic field values ($B = 10^1$, 10^2 , and 10^3) is illustrated in Fig. 4. The critical temperature for hydrogen in a strong magnetic field is virtually identical to the Bose condensation temperature for the ideal Bose gas. The principal difference is attributable to the critical density $n = n_c$ being specific to each B value so that the critical temperature at $n \to n_c$ vanishes due to the strong interaction at a relatively small interatomic distance.



Figure 4. Critical temperature, T_c , of the transition of hydrogen into the superfluid state depending on density, *n*, of the hydrogen gas for three values of *B* (in atomic units): (1) 10, (2) 10^2 , (3) 10^3 .

5. Superfluidity of deuterium in a strong magnetic field

Deuterium atoms in the ground state placed in an ultrahigh magnetic field form the Fermi gas with weak anisotropic interaction, the potential of which is given by Eqn (4.1). It is natural to suppose that deuterium, similar to ³He, should be able to acquire the property of superfluidity when in a strong magnetic field at low temperature [69]. However, pair interaction in the case of deuterium is anisotropic unlike that of ³He which shows isotropic pair interaction but anisotropic superfluid phase [70, 71].

The properties of deuterium at low temperature can be naturally described on the basis of the results of the Bardeen-Cooper-Schrieffer theory (BCS) [71]. In the BCS model, the equation for the order parameter Δ_k at zero temperature has the form

$$\Delta_{k} = -\sum_{k'} \frac{U_{kk'} \Delta_{k'}}{2(\varepsilon_{k'}^{2} + |\Delta_{k'}|^{2})^{1/2}}, \qquad (5.1)$$

where $U_{kk'}$ is the Fourier representation of the potential of the pair interaction and ε_k is the energy of elementary one-particle excitations.

Because deuterium in the strong magnetic field is completely polarised and the spins of all atoms are oriented opposite to the magnetic field lines, the expansion in spherical harmonics near the Fermi surface is likely to contain only those associated with the odd angular momentum:

$$U_{kk'} = b_0 Y_{10}^* (\boldsymbol{\Omega}') Y_{30} (\boldsymbol{\Omega}) + b_0 Y_{30}^* (\boldsymbol{\Omega}') Y_{10} (\boldsymbol{\Omega}) -b_1 Y_{11}^* (\boldsymbol{\Omega}') Y_{31} (\boldsymbol{\Omega}) - b_1 Y_{31}^* (\boldsymbol{\Omega}') Y_{11} (\boldsymbol{\Omega}) -b_1 Y_{1-1}^* (\boldsymbol{\Omega}') Y_{3-1} (\boldsymbol{\Omega}) - b_1 Y_{3-1}^* (\boldsymbol{\Omega}') Y_{1-1} (\boldsymbol{\Omega}) .$$
(5.2)

Here, the solid angles Ω and Ω' describe the directions of the momenta k and k' in the coordinate system with axis zthat parallels magnetic field lines while coefficients b_0 and b_1 are given by

$$b_0 = \frac{64\pi^2}{945\sqrt{21}} k_F^4 U_0 R_0^7 J(k_F R_0) ,$$

$$b_1 = \frac{16\pi^2}{945} \sqrt{\frac{2}{7}} k_F^4 U_0 R_0^7 J(k_F R_0) ,$$

where $k_{\rm F}$ is the value of the momentum on the Fermi surface. Other symbols have the same meanings as in Eqn (4.8). The critical temperature of transition into a superfluid state can be found from the BCS equation for the energy gap, if one bears in mind that its width vanishes at $T \rightarrow T_{\rm c}$.

At $T \neq 0$, the BCS equation for the energy gap can be written in the form

$$\Delta_k(T) = -\sum_{k'} \frac{U_{kk'} \Delta_{k'}(T)}{2E_{k'}(T)} \tanh \frac{E_{k'}(T)}{2k_{\rm B}T}, \qquad (5.3)$$

where $k_{\rm B}$ is the Boltzman constant and

$$E_{\boldsymbol{k}'}(T) = \sqrt{\varepsilon_{\boldsymbol{k}'}^2 + \left| \varDelta_{\boldsymbol{k}'}(T) \right|^2} \; .$$

In the case of the strong anisotropy in question, there are two options for the order parameter to be chosen, according to the angular momentum projection m = 0 or m = 1. It can be shown that the superfluid phase of deuterium is in fact the ground state of the system with the order parameter corresponding to m = 0, which is to be sought for in the form

$$\Delta_{0,\mathbf{k}} = \Delta_0 Y_{10}(\boldsymbol{\Omega}) - \Delta_0 a_1 Y_{30}(\boldsymbol{\Omega}) .$$
(5.4)

Here, a_1 is a constant of the order of unity, and the energy gap is defined by the expression

$$\Delta_0 \approx 2\xi \, \gamma \exp\left(-\frac{4\pi}{b_0 N_0}\right) \,,$$

where $N_0 = mp_F/(2\pi^2\hbar^3)$ is $\frac{1}{2}$ of the density of states on the Fermi surface, $\xi \ll \varepsilon_F$ is the width of the zone in the momentum space near the Fermi surface, and the numerical coefficient

$$\ln \gamma \approx -\frac{1}{2} \int |Y_{10} - Y_{30}|^2 \ln |Y_{10} - Y_{30}| \,\mathrm{d}\boldsymbol{\Omega} = 0.2597 \;.$$

The following expression for the critical temperature can be derived from Eqn (5.4) with the aid of Eqn (5.3):

$$k_{\rm B}T_{\rm c} = 1.14 \,\xi \exp\left(-\frac{4\pi}{|b_0|N_0}\right) \,.$$
 (5.5)

This expression defines the temperature of the transition of deuterium to the superfluid state as a function of gas density. The $T_c(n)$ dependence for the above three magnetic field values ($B = 10^2$, 10^3 , and 10^4) is shown in Fig. 5.



Figure 5. The critical temperature, T_c , of the transition of deuterium into the superfluid state as a function of the density, n, of the deuterium gas for three values of B (in atomic units): $(1)10^2$, $(2)10^3$, $(3)10^4$.

6. Hydrogen molecules in an ultrahigh magnetic field

6.1 A hydrogen molecule in an ultrahigh magnetic field

Hydrogen atoms in a strong magnetic field $(B \gg B_0)$ are completely polarised and their electron spins are oriented against the magnetic field lines, which accounts for the very weak interatomic interaction in the ground state of hydrogen atoms (see the previous section). In this case, the pair-interaction potential associated with the triplet term is characterised by a shallow potential well, while Coulomb repulsion of electrons acquires the role of the dominant factor because of the antisymmetry of the coordinate part of the wave function. At the same time, interatomic distances are relatively large, in accordance with the Pauli principle, which accounts for incomplete overlapping of the electron wave functions and makes it possible to neglect the exchange interaction that falls exponentially with the increasing distance. As regards the quadrupole-quadrupole interaction between atoms, it equally fails to contribute significantly to the interatomic interaction in the triplet term since the potential $U_{qq}(R) \sim 1/R^5$. It has been shown in Sections 3 and 4 that the depth of the potential well in the triplet term is so small as to make possible, in principle, formation of the Bose condensate and transition to the superfluid state,

provided that the temperature is sufficiently low. Conversely, the pair-interaction potential in the singlet term has a very deep potential well facilitating transition to the bound state. However, the energy needed for spin flip of an electron is much higher than the binding energy of the molecule and is even in excess of the atom's ionisation potential.

The situation is quite different in the case of a multielectron system where the excited states of electrons at the lowest Landau level with nonvanishing projection of orbital momentum ($m \neq 0$) acquire greater importance. Unlike the *m*-independent energy of free electrons in the magnetc field, the energy of bound electrons at higher Landau orbitals $(\rho_m = \sqrt{2m + 1}\rho_0)$ increases with growing *m* even though the energy difference between these excited states and the ground state is small compared with the latter's energy. Excitation energy in the state with $m \neq 0$ is asymptotically (at $\ln B \ge 1$) small: $O(1/\ln B_c)$ of the ground state energy. In principle, this situation allows for the atoms to form into molecules of a new type [19, 72] in which "the electron cloud is totally collectivised" (B B Kadomtsev).

Mechanisms of molecular formation in the ultrahigh magnetic field and in its absence are quite different. In a normal hydrogen molecule, the atoms are held together by covalent bonds. Generally speaking, the H_2 molecule can join the third atom only if this atom is excited. In this case, however, the excitation energy is of the same order of magnitude as that of the atom's ground state and as the binding energy in the H_2 molecule which makes formation of such a molecule energetically unfavourable.

Conversely, hydrogen atoms in a strong magnetic field are unable to produce even an H₂ molecule because the interaction between them is weak. Nevertheless, in this situation a hydrogen atom can join an electron of the lowest Landau level with the projection of orbital momentum m = 1 by producing a negative ion H⁻, since the Coulomb repulsion is not very strong for such a configuration. The variation method similar to that mentioned in the beginning of Section 2 may be employed in order roughly to evaluate the binding energy of the H⁻ ion. In other words, the binding energy can be estimated if the minimum of the energy functional is found. With this technique, a binding energy of about $\ln^2 B$ has been obtained. Also, it has been shown with this method that two hydrogen atoms in states m = 0 and m = 1 give rise to a hydrogen molecule which has binding energy in the limit of an ultrahigh magnetic field of the same order $\ln^2 B$.

It should be borne in mind, however, that binding energy estimates thus obtainable are lacking in accuracy because they are derived as the difference between two higher values: the ground state energy of the molecule with 'collectivised' electrons and the combined energy of individual atoms, each value being calculated with only logarithmic accuracy. Binding energy of isolated molecules and long molecular chains has been calculated by many authors [19, 20, 25, 28, 29, 72–74] who used a variety of techniques (variational method, density-functional method, etc.). The Hartree–Fock method proved to yield the best results because it made possible consistent consideration of the exchange interaction [29, 75].

It has been mentioned in the foregoing discussion that binding energy is calculated with logarithmic accuracy. Because the use of the adiabatic approximation implies satisfaction of the inequality $(\ln B)/\sqrt{B} \ll 1$, the results obtained for magnetic fields of practical interest $(B \sim 10^{11} - 10^{12} \text{ G})$ cannot be regarded as reliable. Specifically, for $B_{12} = 10^{12} \text{ G}$, there is only $(\ln B)/\sqrt{B} \approx 0.3$, and the asymptotic expression for the binding energy $\mathcal{E} = -(\ln^2 B)/2$ is attainable only at very high values of the magnetic field, e.g. $B \sim 10^7 B_q \sim 10^{16} \text{ G}$).

Binding energies (dissociation energies) of the hydrogen molecule, H₂, and a chain of molecules, H_n with $n = 3, 4, ..., \infty$ and the molecule axis parallel to the magnetic field lines, was found with the use of the molecular orbital method and the method of Hartree– Fock [75] to calculate the Hamiltonian matrix elements (3.1) proceeding from the respective basic functions.

The Hamiltonian of a chain of n atoms arranged along the z axis at an equal distance a from each other, with the magnetic field **B** oriented along the z axis, has the form

$$\hat{\mathcal{H}} = \hat{H}_B + \hat{H}_{el} + \hat{H}_{ee} + \hat{H}_{II} , \qquad (6.1)$$

where

$$\hat{H}_{B} = \sum_{i=1}^{n} \frac{1}{2m_{e}} \left(\hat{P}_{i} + \frac{e}{c} A_{i} \right)^{2} + \sum_{i=1}^{n} \frac{1}{2} \boldsymbol{\mu} \cdot \boldsymbol{B} , \qquad (6.2)$$

$$\hat{H}_{el} = -\sum_{i,l} \frac{e^2}{|\mathbf{r}_i - la\hat{z}|},$$
(6.3)

$$\hat{H}_{ee} = -\frac{1}{2} \sum_{i \neq j} \frac{e^2}{r_{ij}},$$
(6.4)

$$\hat{H}_{II} = \frac{1}{2} \sum_{I \neq J} \frac{e^2}{a|I-J|} \,. \tag{6.5}$$

Here, symbols i, j and I, J label electrons and ions, respectively.

Assume that all electrons in the ground state are at the lowest Landau level, with their spins directed against the magnetic field. Choose a gauge for the vector potential in the form

$$\boldsymbol{A} = \frac{1}{2} \left(\boldsymbol{B} \times \boldsymbol{r} \right) \,. \tag{6.6}$$

In order to reduce the system of Hartree-Fock equations to a system of one-dimensional equations, represent basic wave functions of one-electron states as

$$\Psi_{n_{\rho}=0,m,\nu}(\rho, \, \varphi, \, z) = \psi_{0,m}(\rho, \, \varphi) \, f_{m,\nu}(z) \,, \tag{6.7}$$

where $\psi_{0,m}(\rho, \varphi)$ are free-electron wave functions at the lowest Landau level (2.7) at $n_{\rho} = 0$ while m = 0, 1, 2..., and $f_{m,\nu}(z)$ are wave functions to be found. For the two-atom H₂ molecule, the wave function $f_{m,\nu}(z)$ may be supposed to have no nodes (quantum number $\nu = 0$) since states with $\nu \neq 0$ have been shown to have by far higher energy (see Section 3).

The normalised antisymmetric electron wave function is given by the determinant of Slater functions (6.7) and, in the case of the two-electron wave function, has the form

$$\Psi(\mathbf{r}_{1}, \mathbf{r}_{2}) = S\{\Psi_{00}(\mathbf{r}_{1}) \Psi_{01}(\mathbf{r}_{2})\}$$

= $\frac{1}{\sqrt{2}}\{\Psi_{00}(\mathbf{r}_{1}) \Psi_{01}(\mathbf{r}_{2}) - \Psi_{00}(\mathbf{r}_{2}) \Psi_{01}(\mathbf{r}_{1})\}, (6.8)$

where the quantum number v = 0 is omitted for the sake of simplicity.

As is known [41], the Hartree–Fock equations follow from the variation principle when the functions Ψ_{00} and Ψ_{01} are varied independently. In order to choose basic functions in the form of Eqn (6.7), it is necessary to average over radial Landau wave functions while the functional $\langle \hat{\mathcal{H}} \rangle$ is varied only with respect to functions f_0 and f_1 . Therefore, the problem in fact is solved in the adiabatic approximation which allows one-dimensional Hartree – Fock equations for functions $f_m(z)$ to be obtained in the form

$$\left[-\frac{\hbar^2}{2m_{\rm e}}\frac{{\rm d}^2}{{\rm d}z^2} - \frac{e^2}{r_0}V_m(z) + \frac{e^2}{r_0}K_m(z) - \mathcal{E}_m\right]f_m(z) = \frac{e^2}{r_0}J_m(z),$$
(6.9)

where m = 0, 1 for the two-atomic molecule, and the potentials averaged over the basic functions are defined as

$$V_m(z) = \int d^2 \rho |\psi_{0,m}(\rho, \varphi)|^2 \sum_I \frac{1}{|r - Ia\hat{z}|}, \qquad (6.10)$$

$$K_m(z) = \sum_{m'} \int dz' \left| f_m(z') \right|^2 D_{m,m'}(z-z') , \qquad (6.11)$$

$$J_m(z) = \sum_{m'} f_{m'}(z) \int dz' f_{m'}(z') f_m(z') E_{m,m'}(z-z'), \quad (6.12)$$

$$D_{m,m'}(z_1 - z_2) = \int d^2 \boldsymbol{\rho}_1 d^2 \boldsymbol{\rho}_2 |\psi_m(\boldsymbol{\rho}_1)|^2 |\psi_m(\boldsymbol{\rho}_2)|^2 \frac{1}{r_{12}}, \qquad (6.13)$$

$$E_{m,m'}(z_1 - z_2) = \int d^2 \rho_1 d^2 \rho_2 \psi_m(\rho_1) \psi_{m'}(\rho_2) \psi_m^*(\rho_2) \psi_{m'}^*(\rho_1) \frac{1}{r_{12}}.$$
(6.14)

For the H₂ hydrogen molecule, the symbols *m* and *m'* in Eqns (6.9)-(6.14) acquire the values of 0 and 1, respectively, while the boundary conditions for the function $f_m(z)$ look like

$$f'_{m}(z=0) = 0 ,$$

$$f_{m}(z \to \pm \infty) \sim \exp\left[-|z| \left(\frac{2m_{e}\rho_{0}^{2}}{\hbar^{2}}|\varepsilon_{m}|\right)^{1/2}\right] .$$
(6.15)

Knowledge of solutions for Hartree-Fock equations (6.9) allows the total H_2 energy to be computed as

$$E = \langle \Psi | \mathcal{H} | \Psi \rangle = \frac{e^2}{a} + \mathcal{E}_{00} + \mathcal{E}_{01} - E^{\text{dir}} - E^{\text{exch}} , \qquad (6.16)$$

where E^{dir} and E^{exch} are the energies of electron – electron and exchange interactions, respectively:

$$E^{\text{dir}} = \int d^3 \boldsymbol{r}_1 d^3 \boldsymbol{r}_2 |\boldsymbol{\Psi}_{00}(\boldsymbol{r}_1)|^2 |\boldsymbol{\Psi}_{01}(\boldsymbol{r}_2)|^2 \frac{e^2}{r_{12}}$$
$$= \frac{e^2}{r_0} \int dz_1 dz_2 \times f_0^2(z_1) f_1^2(z_2) D_{01}(z_1 - z_2) , \quad (6.17)$$

$$E^{\text{exch}} = -\int d^3 \mathbf{r}_1 d^3 \mathbf{r}_2 \times \Psi_{00}(\mathbf{r}_1) \Psi_{01}(\mathbf{r}_2) \Psi_{00}^*(\mathbf{r}_2) \Psi_{01}^*(\mathbf{r}_1) \frac{e^2}{r_{12}}$$
$$= -\frac{e^2}{r_0} \int dz_1 dz_2$$

$$\times f_0(z_1) f_1(z_2) f_0(z_2) f_1(z_1) E_{01}(z_1 - z_2) , \qquad (6.18)$$

At $\alpha \to \infty$, the total energy (6.16) must undergo transformation to the sum of energies of individual atoms



Figure 6. The size (a), and the binding energy (b) of a hydrogen molecule for the bound molecular state $(\mathcal{E}_{01}, R_{01})$ and for singlet $(\mathcal{E}_{00S'} R_{00S})$ and triplet $(\mathcal{E}_{00T} R_{00T})$ terms of the ground state of the atoms.

in the ground state \mathcal{E}_{00} (at m = 0) and in the excited state \mathcal{E}_{01} (at m = 1).

The binding (dissociation) energy of the H₂ molecule is reported [75] to have been found from a numerical solution by means of the molecular orbital method and from numerical solution of the Hartree-Fock equation (6.9). The field-dependent molecule (H_2) size and binding energy values \mathcal{E}_{01} as obtained in Ref. [75] are shown in Fig. 6. For comparison, this figure also presents the binding energy (the depth of the potential well) and the size (minimum in the potential of interatomic interaction) of the H₂ molecule for triplet $(\mathcal{E}_{00T}, R_{00T})$ and singlet $(\mathcal{E}_{00S}, R_{00S})$ terms when both hydrogen atoms occur in the lowest state $(n_o = 0, m = 0)$ v = 0) [61]. Specifically, dissociation energy of the H₂ molecule for the magnetic field $B = 10^{12} \,\mathrm{G}$ is $\mathcal{E}_{01} = 45.4 \text{ eV}$ and its size is $R_{01} = 0.24 a_0$ [75] whereas the binding energy in the triplet term is $\mathcal{E}_{00T} = 1$ eV and the size of the 'molecule' is $R_{00T} \approx 0.4 a_0$. For the singlet term the binding energy is $\mathcal{E}_{00S} = 1$ keV and the size is $R_{00S} \approx 0.1 a_0$. Energies of the ground state (m = 0) and the first excited state (m = 1) of the hydrogen atom are -161 eV and -117 eV, respectively.

6.2 Formation of large polymeric hydrogen molecules

It has already been noted that in a vanishing magnetic field, the hydrogen molecule (H₂) is formed because of covalent bonding, which makes addition of another hydrogen atom energetically unfavourable. The situation is quite different in an ultrahigh magnetic field since the energy difference between excited states with $m \neq 0$ at the lowest Landau level is insignificant as compared with the ground state energy $n_{\rho} = 0$, m = 0. In this case, atoms are

likely to draw together even if they are completely polarised (see Section 3), and the formation of large hydrogen molecules H_n with $n \ge 1$ may prove energetically preferable.

At large distances, atoms are believed to have the shape of thin needles oriented parallel to the magnetic field lines and interact as quadrupoles. For distribution of electron density $n_e \sim exp(-2\alpha|z|)$, the energy of the quadrupole– quadrupole interaction with momentum $Q_{qq} = 2\langle z^2 \rangle = \alpha^2/2$ is

$$Q_{qq} = \frac{9}{8} \frac{1}{\ln^4 B} \frac{1}{R^5} P_4(\cos\theta) .$$
 (6.19)

if the interatomic distances are greater than the atom's size. When on one line, atoms may be either reciprocally repulsive or attractive (at $\theta = 0, \pi$ and $\theta \approx 49^{\circ}$ respectively). The potential of the quadrupole-quadrupole interaction progressively decreases at greater distances, which allows the interaction at $R \ge 1/\alpha$ to be neglected.

When atoms draw together, the electrons are 'collectivised' and occupy the lowest levels associated with longitudinal (along the magnetic field) motion. Owing to this, n atoms ($n \ge 1$) placed in an ultrahigh magnetic field form a molecule which is extended parallel to the field lines and has an electron shell radius (in the plane perpendicular to the magnetic field) identical with the maximum Landau orbit radius

$$R_n \approx \sqrt{2n-1} \rho_0 \approx \sqrt{\frac{2n}{B}}$$
.

(The electrons are assumed sequentially to fill in orbits with m = 0, 1, ..., n - 1.) To estimate the binding energy of such a molecule, the variation method used in Ref. [72] to calculate the energy of a two-atom molecule of heavy atoms in an ultrahigh magnetic field $(B \ge 2Z^3)$ may be applied. Similar numerical calculations of binding energy by the method of Hartree-Fock were reported in Ref. [75] for the H_n molecule comprising n hydrogen atoms.

If the exchange interaction is disregarded, the energy of the molecule of *n* hydrogen atoms interacting at distances *a* may be approximately presented as a sum of electron kinetic energy and Coulomb energy V_{ee} , V_{eI} , and V_{II} :

$$E = n \int d^3 \boldsymbol{r} \left[\frac{1}{2} \left(\frac{\partial \boldsymbol{\Psi}}{\partial z} \right)^2 + \frac{n-1}{2} \left\langle \frac{1}{r} \right\rangle \boldsymbol{\Psi}^2 - \sum_{I=-n/2}^{n/2} \frac{1}{|\boldsymbol{r}-al\hat{z}|} \boldsymbol{\Psi}^2 \right] + \sum_{I(6.20)$$

Here, Ψ^2 is the average wave function normalised by the condition $n\Psi^2 = n_e$ (where mean electron density $n_e = \sum_i \Psi_i^2$) and

$$\left\langle \frac{1}{r} \right\rangle = \int \mathrm{d}^3 \mathbf{r}' \frac{1}{|\mathbf{r} - \mathbf{r}'|} \Psi^2(\mathbf{r}') \;.$$
 (6.21)

The ground state energy can be estimated from minimising the functional (6.20), subject to the additional constraint

$$\int \mathrm{d}^3 \boldsymbol{r} \, \boldsymbol{\Psi}^2(\boldsymbol{r}) = 1 \; .$$

Bearing in mind that a molecule in an ultrahigh magnetic field has the shape of a thin needle of length $L \sim na \gg R$ and electron density outside atoms vanishes as

 $\exp(-2\alpha|z|)$ along the z axis and as $\exp(-\rho^2/R^2)$ radially, one takes test functions from

$$\Psi^{2}(\mathbf{r}) = \frac{\alpha}{\pi R^{2}} \exp\left\{-2\alpha |z| - \frac{\rho^{2}}{R^{2}}\right\} , \qquad (6.22)$$

where α is the free parameter. Substitution of (6.22) into Eqn (6.20) gives, with logarithmic accuracy, the following expression for the energy:

$$E \approx n \left\{ \frac{\alpha^2}{2} + 2n\alpha \ln(\alpha R) - \frac{1}{2}n\alpha \ln(\alpha R) + \sum_{I=1}^{n/2} \frac{1}{aI} \right\}.$$
 (6.23)

The energy per atom can be presented as [75]

$$\frac{E}{n} \approx \frac{\alpha^2}{2} - \frac{3}{2} n\alpha \ln \frac{2}{n\alpha R} + \frac{3}{2} n\alpha \gamma , \qquad (6.24)$$

where $\gamma = 0.577$ is the Euler constant.

Variation with respect to α yields

$$\alpha = \frac{3}{2}nl,$$

$$l = \ln \frac{2}{n\alpha R} \approx \ln \sqrt{\frac{B}{n^5}},$$

$$\frac{E}{n} \approx -\frac{9}{8}n^2 \ln^2 \sqrt{\frac{B}{n^5}},$$
(6.25)

where $\alpha R \ll 1$ and $\ln(2/n\alpha R) \gg 1$.

It is worthwhile to note that the solution for the 'long' hydrogen molecule thus obtained is in a way equivalent to the approximate solution for a heavy atom in a high magnetic field [76, 77] (see also Section 7). The distance between atomic nuclei rapidly decreases with increasing *n*; therefore $\alpha = (4/9n^2) \ln^{-1} \sqrt{B/n^5}$.

The ground state energy of the H₂ molecule can be estimated from simple qualitative considerations similar to those described in [19]. Suppose that *n* hydrogen atoms are situated on the *z* axis at similar distances α . The molecule length and radius are $L \approx na$ and $R \approx \sqrt{2n/B}$, respectively, and it is assumed that $n \gg 1$ and $L \gg R$. Treating the molecule as a thin, uniformly charged cylinder with radius *R* and length *L* yields, with logarithmic accuracy, the following expression for the total energy, i.e. the sum of kinetic and potential energies:

$$E \approx n \left(\frac{p_z^2}{2m_e} + U\right) \approx n \left(\frac{1}{L^2} - \frac{n}{L} \ln \frac{2a}{R}\right) .$$
 (6.26)

Variation of Eqn (6.26) with respect to L gives

$$L \approx \frac{1}{nl}, \quad E \approx -n^3 l^2, \qquad (6.27)$$

where

$$l = \ln \frac{2a}{R} \approx \ln \frac{B^{1/2}}{n^{5/2} \ln B}$$

It should be emphasised that these expressions for the hydrogen molecule energy are only asymptotic and valid only under the strong condition $\ln B \ge 1$. Numerical calculations indicate that the asymptotic formulas are actually correct only at $B \ge 10^7$.

A rise in *n* is accompanied by electrons in the molecular shell of H_n occupying progressively higher orbits $R \approx \sqrt{2n-1} \rho_0$ until saturation corresponding to $n = n_s$ is achieved at $R \sim a$. From $n \ge n_s$ on, filling states which correspond to wave functions with nodes in z, i.e. $v \ne 0$, becomes energetically favourable. It is evident [19, 75] that in the limit $n \ge n_s \ge 1$ the energy of a uniformly charged cylinder with radius R does not depend on n and is

$$E = -0.39 B^{2/5} = -10.6 \left(\frac{B}{B_9}\right)^{2/5} \text{ eV},$$
 (6.28)

while

$$R \approx \frac{1.7}{R^{2/5}}, \quad a \approx 1.88 R$$
 (6.29)

It should once again be emphasised that all these formulas are valid only if considered as distant asymptotics at $B \ge 1$, and even for the magnetic field $B = 10^{12}$ their accuracy is no better than an order of magnitude.

In the numerical calculation of binding energy for H_n molecules at $n = 2, 3, ...\infty$ reported in Ref. [75], the electron density was assumed to be uniform along the *z* axis, and products of plane waves in *z* and Landau functions $\Psi_{0,m}(\rho, \varphi)$ served as basic functions. The binding energy \mathcal{E}_{∞} for H_{∞} molecules, dissociation energy $\mathcal{E}_{\infty}^{dis}(H_{\infty+1} \to H_{\infty} + H)$, and equilibrium distance between atoms as functions of the magnetic field strength as obtained in Ref. [75] are shown in Fig. 7.



Figure 7. Binding energy \mathcal{E}_{∞} , dissociation energy $\mathcal{E}_{\infty}^{\text{dis}}$, and interatomic distance for the infinite molecule chain of hydrogen atoms as functions of the strength , *B*, of the magnetic field.

Note that the order of magnitude of the number of molecules formed in the atmosphere of a neutron star is determined by the small ratio $(k_{\rm B}T/\ln^2 B)$. The number of molecules both on the star's surface and in its atmosphere at a surface temperature of around 10 eV should be great if the dissociation energy of hydrogen molecules in the case of $B = 10^{12}$ G ranges from 46 eV for H₂ to 29 eV for H_{∞} as was calculated in Ref. [75]. The presence of a large number of molecules must influence the cooling rate of the star and can be revealed in the analysis of UV and x-ray spectra.

However, it should be emphasised that the binding energy for a hydrogen molecule and for the H_n molecule calculated in Ref. [75] can be considered only as a tendency to form a molecular state. These authors used the adiabatic approximation in order to reduce the problem to onedimensional Hartree–Fock equations. The accuracy of this method is rather low, especially in the region of fields B < 500. Second, methods based on the use of atomic

orbitals as a first approximation to set up an approximate solution for any system with exchange interaction, for instance the Heitler-London method, yields wrong results at large separations (see the detailed discussion in Refs [41, 62, 63]. As a matter of course, when the authors of Ref. [75] employed the molecular-orbital and HF methods to calculate the interaction energy of the molecule, they also came to this. To resolve the difficulty, they were forced to employ an artificial approach based on the idea of configuration interaction (a detailed critique of these methods may be found in Ref. [63]). There is also another serious shortcoming in the calculations in Ref. [75]. The minimum of the interaction energy of the molecule found there lies at interatomic distances a greater than or equal to the atomic size α in fields 1 < B < 300. The quadrupole forces $\approx 4.5 \alpha^4 P_4(\cos \theta)/a^5$, where θ is the angle between the molecular axis and the field, acting between atoms at all $a \ge \alpha$ are of the same order as the dissociation energy D_2 calculated in Ref. [75], and these forces become repulsive, destroying the 'accuracy' of calculation, when the molecular axis coincides with the magnetic field direction. Thus, the picture of interaction presented in Ref. [75] needs serious revision.*

7. Heavy atoms in strong magnetic fields. The Thomas – Fermi model

The problem of binding energy and ionisation energy of a heavy atom with $Z \ge 1$ is one of the most important to solve if the surface structure of neutron stars is to be understood. Calculation of the multielectron system for this purpose by the Hartree-Fock method is cumbersome. For this reason, the simpler method of Thomas-Fermi [41] is used in the case of heavy atoms even though it is far less precise than the previous one. Properties of heavy atoms and molecules in the ultrahigh magnetic fields thought to be inherent on the surface of neutron stars were first examined in Refs [19, 43, 72, 73, 76, 77]. More extensive studies were the subjects of further reports [57, 58, 78-81]. Evidently, the accuracy of the Thomas-Fermi approach increases as the number of electrons rises, that is at higher Z. Indeed, it has rigorously been demonstrated that the Thomas-Fermi model is asymptotically accurate in the limit $n_e \to \infty, Z \to \infty$. This appears to be equally true of heavy atoms $(Z \to \infty)$ in an ultrahigh magnetic field [84]. Mathematical aspects of this model in the limit $Z \to \infty, B \to \infty$ have been discussed in Refs [84-86].

For the case of heavy atoms $(Z \ge 1)$, the definition of ultrahigh magnetic field needs to be made more specific. If the total number of electrons is denoted by N and the nuclear charge by Z, then N < Z and N = Z correspond to positive ion and neutral atom, respectively. There are no solutions that describe negative ions N > Z and bound molecular states in the Thomas-Fermi model [87-89]. Electrons in the ground state in a strong magnetic field are located on cyclotron orbits with radii $\rho_m = \sqrt{2m + 1}\rho_0$ where m changes from m = 0 to $m = m_{\text{max}}$. The spins of all electrons are directed against the magnetic field lines since $B \ge 1$. A magnetic field may be considered strong provided

$$\rho_m \ll \frac{a_0}{Z} \,. \tag{7.1}$$

†Paragraph added in proof of English edition.

If condition (7.1) is satisfied for $m_{\max} \ge N$, i.e. for all m including $m_{\max} = Z$, filling the lowest Landau level alone becomes energetically favourable. In this case, electron motion along the z-axis corresponding to the ground state can be described by wave functions which have no zeros in z. Electrons fill up cyclotron orbits from m = 0 to m = N, and the electron shell of the atom is markedly extended along the magnetic field lines. The ultrahigh magnetic field condition corresponding to condition (7.1) has the form

$$B \gg 2Z^3 . \tag{7.2}$$

Strictly speaking, it is necessary to distinguish between the following strength ranges of the magnetic field [84]:

(1)
$$B \ll Z^{4/3}$$
,
(2) $B \approx Z^{4/3}$,
(3) $Z^{4/3} \ll B \ll Z^3$,
(4) $B \approx Z^3$,
(5) $B \gg Z^3$. (7.3)

In ranges (1), (2), and (3), electron density exhibits spherical symmetry. Electrons in ranges (3), (4), and (5) are at the lowest Landau level. Atoms in ranges (4) and (5) appear to be markedly extended parallel to the magnetic field lines rather than appearing to be spherical. The ranges of moderately high (3) and ultrahigh (5) magnetic fields are believed to be of primary importance to the physics of neutron stars. Respective numerical values of the magnetic field in the case of iron (Z = 26) are

$$B = 26^{4/3}B_9 = 1.8 \times 10^{11} \text{ G}, \quad B = 26^3B_9 = 4.1 \times 10^{13} \text{ G}.$$

7.1 Heavy atom in a moderately strong magnetic field

Let us examine the moderately strong magnetic field assuming that $M_{\text{max}} \ll N, Z$. In this case, electrons are at the lowest Landau level. Because the width of the wave functions $\psi(\rho) \sim \exp(-\rho^2/B)$ is of the order of $1/\sqrt{B}$, the wave functions of adjoining cyclotron orbits are likely to overlap unless B is too high. In this situation, the filling of excited levels with small m values becomes energetically favourable. Respective wave functions $f_{\nu}(z)$ with $\nu \neq 0$ have zeros, while electron density is more or less uniform along the z-axis. Each m level in the ground state is occupied by at least several electrons, which allows for the Thomas-Fermi approximation to be used. In the adiabatic approximation, the number of electron states in the phase space is easy to evaluate if one takes into account that the radius of the cyclotron orbit in the plane perpendicular to the magnetic field lines is $\rho_m \approx \sqrt{2m/B}$, that is the number of possible 'transverse' states $dN_{\perp} \equiv dm = \rho B d\rho$. The motion of an electron along the magnetic field within the adiabatic approximation is assumed to be one-dimensional with momentum p_z ; so that $\mathrm{d}N_{||} = p_z \,\mathrm{d}z/2\pi.$

Hence, the total number of states in the elementary cell is

$$\mathrm{d}N_{\perp}\,\mathrm{d}N_{\parallel} = \frac{p_z B}{2\pi}\,\rho_m\,\mathrm{d}\rho_m\,\mathrm{d}z = n_\mathrm{e}(\mathbf{r})\,\pi\rho\,\,\mathrm{d}\rho\,\,\mathrm{d}z\,\,, \tag{7.4}$$

from which it ensues that the electron density is

$$n_{\rm e}(\mathbf{r}) = \frac{B}{2\pi^2} p_z$$
 (7.5)

The total kinetic energy of the electrons inside the Fermi surface is

$$K[n_{\rm e}(\mathbf{r})] = \,\mathrm{d}N_{\perp} \frac{\mathrm{d}z}{2\pi} \int_{|p| \,\leq\, p_{\rm F}} \frac{p^2}{2} \,\mathrm{d}p \,\,, \tag{7.6}$$

This, with the use of Eqn (7.5), leads to the kinetic energy density:

$$k(\mathbf{r}) = \frac{2\pi^4}{3B^2} n_{\rm e}^3(\mathbf{r}) .$$
 (7.7)

If one neglects the exchange interaction, the Thomas– Fermi equations are implied by the minimum condition for the total energy functional:

$$E = \frac{2\pi^4}{3B^2} \int n_{\rm e}^3(\mathbf{r}) \,\mathrm{d}^3\mathbf{r} - Z \int \frac{n_{\rm e}(\mathbf{r})}{r} \,\mathrm{d}^3\mathbf{r} + \frac{1}{2} \int \frac{n_{\rm e}(\mathbf{r})n_{\rm e}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \,\mathrm{d}^3\mathbf{r} \,\mathrm{d}^3\mathbf{r}'$$
(7.8)

subject to the additional normalisation constraint

$$N = \int n_{\rm e}(\mathbf{r}) \, \mathrm{d}^3 \mathbf{r} \, . \tag{7.9}$$

Variation of Eqn (7.8) gives the relation which expresses electron density in terms of the electrostatic field potential:

$$n_{\rm e}(\mathbf{r}) = \frac{B}{2\pi^2} \sqrt{2(\varphi - \varphi_0)} .$$
 (7.10)

This relation follows explicitly from the energy conservation law $p_z^2/2 = \varphi - \varphi_0$, where the electrostatic potential is defined as

$$\varphi(\mathbf{r}) = -\frac{Z}{r} + \int \frac{n_{\rm e}(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} \, \mathrm{d}^3 \mathbf{r}' \,. \tag{7.11}$$

It will be recalled (see Ref. [41]) that φ_0 is the maximum energy; moreover, $\varphi_0 > 0$ and $\varphi_0 = 0$ for ion and neutral atom, respectively.

Substitution of expression (7.10) into the Poisson equation,

$$\nabla^2 \varphi(\mathbf{r}) = -4\pi n_{\rm e} , \qquad (7.12)$$

gives the final equation for φ in the form

$$\nabla^2 \varphi(\mathbf{r}) = -\frac{2B}{\pi} \sqrt{2(\varphi - \varphi_0)}.$$
(7.13)

The latter equation is spherically symmetric [57, 76], that is both its solution $\varphi(\mathbf{r})$ and the function $n_{\rm e}(\mathbf{r})$ which minimises the energy functional (7.8) depend only on $r = |\mathbf{r}|$. Natural boundary conditions for $\varphi(r)$ imply that at $r \to 0$, the potential $\varphi(r)$ tends to the Coulomb potential of the nucleus with charge Z:

$$\lim_{r \to 0} r\varphi(r) = -Z , \qquad (7.14)$$

whereas at $r \to \infty$, the potential $\varphi(r)$ must decrease at least faster than 1/r because of screening of the nucleus by the shell electrons.

It is convenient to introduce a new variable x and function χ , instead of r and $\varphi(r)$:

$$x = r \left(\frac{2^3 B^2}{\pi^2 Z}\right)^{1/5}, \quad \chi(x) = -\frac{r}{Z} [\varphi(r) - \varphi_0] . \tag{7.15}$$

In the variables defined in Eqns (7.15), Eqn (7.13) and the boundary conditions take the form

$$\chi''(x) = \sqrt{x\chi} \quad (7.16)$$

$$\chi(0) = 1, \quad \chi(x \to \infty) = 0.$$
 (7.17)

The case of the positive ion (N < Z) requires additionally that the condition $\chi(x_0) = 0$ be satisfied on the ion's boundary (with $x = x_0$). Taking into account this condition, one can obtain from Eqns (7.9) and (7.16),

$$N = Z \int_0^{x_0} \frac{\mathrm{d}}{\mathrm{d}x} \left[x \chi'(x) - \chi(x) \right] \mathrm{d}x = Z \left[1 + x_0 \chi'(x_0) - \chi(x_0) \right].$$
(7.18)

Because Eqn (7.16) and boundary conditions (7.17) in the variables x and χ are independent of N and Z, the transformation formulas to the new variables of Eqns (7.15) may be considered to determine the universal dependence of the atomic radius, potential, and electron density on the nuclear charge Z and the magnetic field. Knowledge of solutions of Eqn (7.16) allows electron density, atomic energy, and ionisation energy to be expressed in terms of $\chi(x)$. Representation of φ in terms of $\chi(x)$ in Eqn (7.10) gives for the electron density,

$$n_{\rm e} = \left(\frac{2}{\pi^{11}}\right)^{1/5} Z^{2/5} B^{6/5} \left[\frac{\chi(x)}{x}\right]^{1/2} . \tag{7.19}$$

With Eqn (7.19) taken into account, the total atomic energy can be written as [78]

$$E = -\left(\frac{8}{\pi^2}\right)^{1/5} Z^{9/5} B^{2/5} \left[\chi'(0) + \frac{1}{x_0} \left(1 - \frac{N}{Z}\right)^2\right], \quad (7.20)$$

while the ionisation energy is considered to be the energy difference:

 $E_{\rm I} = E(Z, N-1) - E(Z, N)$.

Therefore, atomic radius and atomic energy in a moderately strong magnetic field depend on Z and B as

$$R(Z, B) \propto Z^{1/5} B^{-2/5}, \quad E(Z, B) \propto -Z^{9/5} B^{2/5}.$$
 (7.21)

The range of a moderately strong magnetic field is determined by the applicability of the Thomas-Fermi method together with the method of adiabatic approximation used to find the solution. Therefore, it is necessary that the Coulomb interaction in the atom should be small compared with the gap between the Landau levels, i.e. $Z/R \ll \hbar\omega_c$. Since the characteristic atomic size $R \propto Z^{1/5}B^{-2/5}$ [in compliance with Eqn (7.15)], a limit on the magnetic field $B \ll Z^{4/3}$ can be obtained. At the same time, for the Thomas-Fermi model to be applicable, the Fermi length of the electron wave must be small compared with the atom's size. The condition that the magnetic field should be moderately strong means that each level with the quantum number *m* is occupied by at least several electrons, i.e. $\rho_Z \gg 1/Z$. Hence, with $\rho_Z \approx \sqrt{2Z/B}$, it follows that $B \ll Z^3$. Therefore, situations to which solutions in the Thomas-Fermi model may be applied are defined by the relation

$$Z^{4/3} \ll B \ll Z^3 . \tag{7.22}$$

The Thomas-Fermi method is known to be especially convenient because it allows simple analytic solutions to be obtained. However, its accuracy is significantly lower than that of other techniques, e.g. the Hartree-Fock method. The lack of accuracy in the Thomas-Fermi method in the case of a strong magnetic field can be accounted for by at least two factors: its inability to take into consideration the exchange interaction and the use of the adiabatic approximation. It is known that the exchange interaction effectively diminishes the electrostatic repulsion of electrons, which results in their higher density in the shell than is predicted by the simple Thomas-Fermi model. This, in turn, makes the radius of the atom smaller and enhances its energy. Results of numerical calculation in the framework of the Thomas-Fermi-Dirac model as reported in Ref. [78] indicate that the relative contribution of the exchange interaction (especially to ionisation energy) may be of the order of 30% - 60% depending on Z, N, and B. When the exchange interaction is taken into account, the total binding energy of the atom rises while its radius becomes smaller. However, the relative contribution of the exchange interaction to binding energy and ionisation energy decreases as the magnetic field grows.

The inaccuracy of the Thomas-Fermi method related to the use of the adiabatic approximation in calculating kinetic energy as the electron density functional has been discussed in Ref. [79]. More exact calculations of the electron density [79, 90] were reported to lead to an equation for the potential which [even if spherically symmetric as in Eqn (7.16)] explicitly contains parameters Z and B in both the equation and the boundary conditions; from this point of view, the scaling of expressions (7.21) is approximate and asymptotically exact at $B \to \infty$. According to numerical calculations in Ref. [79], the solution at $B = (10-50)B_9$ is at variance with that obtained in the adiabatic approximation, but at $B \ge 1000B_9$ the results are in good agreement with the adiabatic approximation.

7.2 Heavy atom in an ultrahigh magnetic field

When $m_{\text{max}} \ge N$, condition (7.2) for an ultrahigh magnetic field is fulfilled. In this case, electrons are at the lowest levels (with respect to azimuthal quantum number m) of cyclotron orbits in the lowest Landau zone, each occupying one level. The atom is elongated parallel to the magnetic field lines, and its shell radius is comparable with the radius of the maximal cyclotron orbit $\rho_Z \approx \sqrt{2Z/B}$. Under these conditions, the ground state of a heavy atom is analogous to that of a hydrogen atom at $B \ge 1$. The energy of a heavy atom can be computed in the mean field approximation [77], following the approach used in Section 6.2. It is clear from what was said at the end of Section 7.1 that the adiabatic approximation in the case in question must ensure sufficient accuracy and requires no significant correction for the exchange interaction. By analogy with expression (6.20), the atomic energy is found as

$$E = \int d^3 \boldsymbol{r}_1 \dots d^3 \boldsymbol{r}_N \left\{ \frac{1}{2} \sum_i \left(\frac{\partial \boldsymbol{\Psi}}{\partial z_i} \right)^2 - \sum_i \frac{Z}{r_i} \boldsymbol{\Psi}^2 + \frac{1}{2} \sum_{i \neq j} \frac{1}{|\boldsymbol{r}_i - \boldsymbol{r}_j|} \boldsymbol{\Psi}^2 \right\}.$$
 (7.23)

If the exchange interaction is neglected, the wave function Ψ is merely the product of one-particle electron wave functions in a self-consistent electric field, and the energy is

expressed in terms of the mean electron density $n_e = \sum_i \Psi_i^2$. This leads to an equation similar to Eqn (6.20):

$$E = N \int d^3 \boldsymbol{r} \left[\frac{1}{2} \left(\frac{\partial \boldsymbol{\Psi}}{\partial z} \right)^2 + \frac{N-1}{2} \left\langle \frac{1}{r} \right\rangle \boldsymbol{\Psi}^2 - \frac{Z}{r} \boldsymbol{\Psi}^2 \right]. \quad (7.24)$$

Here, Ψ is the mean wave function normalised by the condition $N\Psi^2 = n_e$ while $\langle 1/r \rangle$ is given by Eqn (6.21).

Similar to Section 6.2, the wave function may be chosen in the form of Eqn (6.22). Substitution of Eqn (6.22) into Eqn (7.24) yields, with logarithmic accuracy,

$$E \approx \frac{N\alpha^2}{2} - 2NZ \ln (\alpha R) + \frac{1}{2}\alpha N(N-1)\ln (\alpha R) , \quad (7.25)$$

where $R = \rho_N$ and $\alpha \rho_N \ll 1$.

Variaton of expression (7.25) with respect to α gives, from the energy minimum condition with logarithmic accuracy [77],

$$\alpha = \frac{1}{2}(4Z - N + 1)L ,$$

$$E = -\frac{N}{8}L^{2}(4Z - N + 1)^{2} .$$
(7.26)

The expression for L in Eqns (7.26) is similar to the expression for l in Eqn (6.25) and, when N = Z, has with logarithmic accuracy the form

$$L \approx \frac{1}{2} \ln \frac{B}{Z^3} \,. \tag{7.27}$$

To sum up, both the shape of the heavy atom and the expression for energy in an ultrahigh magnetic field $B \ge Z_3$ are similar to the respective characteristics of the hydrogen atom at $B \ge 1$. Specifically, the formula for energy (7.26) at Z = N = 1 tends to the asymptotic formula for the binding energy of a hydrogen atom $\mathcal{E}_{\rm H} = (\ln^2 B)/2$. The ionising energy of a neutral atom,

$$E_1 = \frac{3}{8}L^2 Z^2 , \qquad (7.28)$$

grows rapidly with increasing Z, unlike the ionisation energy in a moderately strong magnetic field. It should be emphasised that the numerical value of the ionisation energy for heavy atoms with $Z \ge 1$ amounts to hundreds of kiloelectron-volts and appears to be enormously high if judged by 'terrestrial criteria'.

7.3 Molecules. Equations of state

The cooling rate of a neutron star depends on the state of its matter, density profile, and temperature gradient in the surface layer. It is therefore important to know the equation of state for the matter on the stellar surface in a strong magnetic field.

By virtue of the simplicity of the Thomas–Fermi model, it is tempting to extend its use to studies of bound molecular states and the equation of state, in spite of the low accuracy of the model as compared with that provided by the mean field approximation method.

The results of such an approach have been reported in a review [81] and in Refs [91–94], and only a few more general observations as regards applicability of the Thomas- Fermi method seem to be appropriate in the following discussion.

In its simplest form (i.e. ignoring exchange interaction between electrons), the Thomas-Fermi equation can be derived by variation of the total energy functional [see expression (7.8)] to which a term describing the Coulomb interaction between nuclei should be added. Introduction of the exchange interaction does not result in any substantial complication. The equation of state for cold matter in a strong magnetic field, with the exchange interaction taken into account (Thomas-Fermi-Dirac model), has been considered in Refs [81, 92].

As is known, neither the Thomas–Fermi approach nor the Thomas-Fermi-Dirac model have solutions corresponding to stable bound molecular states. In this context, there is no solution corresponding to the condensed state with zero pressure. The statement of the absence of solutions corresponding to stable molecules in the Thomas-Fermi model (known as the Teller theorem [88, 89]) is evident from the fact that in the Thomas-Fermi approximation, the atomic energy and the radius of the atom are proportional to $Z^{7/3}$ and $Z^{-1/3}$, respectively, while the binding energy of the molecules and their size dependent on the electrons in the external shell of the atom must be unrelated to the nuclear charge or show only a weak relation. The problem may be posed in a more general context as the problem of matter stability (see the discussion in Refs [95, 96]). It is possible to evaluate the exchange energy of molecules in the modified Thomas-Fermi-Dirac-Weitszeker model, which takes into account terms with the electron density gradient in the kinetic energy functional. Estimates of molecular binding energy in a strong magnetic field on the basis of the modified model [94] agree qualitatively with the results obtained by the mean field approximation method.

8. Matter in ultrahigh magnetic fields

The problem of the binding energy of the matter in a strong magnetic field on the surface of a neutron star appears to be of primary importance for the theory of the pulsar magnetosphere. The matter may either exist in the solid phase, giving rise to a one-dimensional metallic lattice, or form the liquid (gaseous) layer on the stellar surface, depending on whether the value of the binding energy is high or low. The mode of existence dictates boundary conditions for the electric field at the surface of the pulsar, which provide the basis for a variety of theoretical models of the magnetosphere [22, 24, 33, 34, 97].

There is a choice between a magnetosphere model with free emission of particles from the star and that with trapped emission and finite electric field on the stellar surface. The specific field value at the surface is a function of temperature. However, it shows even greater dependence on the binding energy of the surface matter, thermal emission being the prevalent process. The thermoemission constant is difficult to calculate in this situation. Nevertheless, it is concluded that, on the basis of extrapolation of thermoemission rates attainable in the laboratory, the minimum binding energy of the matter compatible with the models of a magnetosphere with finite electric field is $E_{\rm min} \approx 3 \, \rm keV$ at a surface temperature of 100 eV.

Crystal structures in the solid phase with optimal binding energy are possible because of the cylindrical shape of the atoms in an ultrahigh magnetic field. Therefore, they should be expected to be either body-centered tetragonal (D_{4h}) or rhombohedral (D_{3d}) lattices. What is actually needed is a reasonably reliable estimation of the binding energy of an infinitely long chain of molecules.

In earlier studies [20, 98], the binding energy of polymeric molecules was calculated on the assumption that long molecules are densely packed because of adhesion, giving rise to solids. Typical values of binding energy obtained in Refs [20, 98] for the crystal lattice of iron atoms were found to range from 2.6 keV for $B = 10^{12}$ G, to 10 keV for $B = 5 \times 10^{12}$ G. However, more accurate calculations [99] demonstrated that these values are overstated by approximately one order of magnitude.

Simple estimates of the atom's binding energy in a crystal lattice placed in a strong magnetic field (see, for instance, those in Section 6.1) are not in the least bit reliable since they have been calculated on the assumption that binding energy in a crystal lattice is the difference between two large numbers, each obtained with insufficient accuracy. Generally speaking, it is a priori evident that singlet terms responsible for strong interatomic bonding energy must be effective because atoms in an ultrahigh magnetic field are completely polarised. Therefore, the binding energy must be small. This inference is confirmed by numerical calculations of binding energy on the basis of either the density functional method [25-27] or the Hartree–Fock approach [28, 29].

Attempts to calculate the binding energy for bodycentered tetragonal and rhombohedral crystal lattices of iron atoms in a strong magnetic field have been reported in Refs [25–27]. Electrons were supposed to show exchange interaction as if they formed a homogeneous gas in the absence of a magnetic field. The binding energy of the bodycentered lattice thus obtained turned out to be no more than 0.12 keV for $B = 10^{12} \text{ G}$ and 0.5 keV for $B = 5 \times 10^{12} \text{ G}$.

A more consistent account of the exchange interaction is available in the Hartree–Fock model. However, calculation of the binding energy of a crystal lattice remains a cumbersome and tedious task. Binding energy values for molecule chains calculated in the Hartree–Fock approximation [28, 29] indicate that heavy atoms do not produce bound states in a strong magnetic field. It has been shown that isolated atoms are energetically more preferable than chains of molecules [29]. This is true for atoms with Z > 2in a magnetic field $B > 10^{12}$ G and for atoms with Z > 4 in a magnetic field $B > 5 \times 10^{12}$ G. The binding energy of the molecule of helium atoms found in Ref. [29] is about 25 eV per atom at $B = 10^{12}$ G, while atoms with $Z \ge 3$ at $B > 10^{12}$ G do not assemble into chains at all.

Evaluation of binding energy for a polymeric molecule of iron atoms in a strong magnetic field in the Hartree– Fock approximation yields values below 1 keV, while possible binding energy between polymeric chains is less than 0.5 keV [29]. To sum up, the calculations indicate that in both the density functional approximation and the Hartree–Fock approximation, heavy atoms do not form the bound states in ultrahigh magnetic fields.

9. Conclusion

The physical properties of matter have been shown to change drastically in the presence of an ultrahigh magnetic field. In particular, the electron shell structure of the atom is subject to radical alteration. Atoms show marked lengthwise extention along the magnetic field lines, with their binding energy and ionisation potential being substantially increased. Concurrently, there is a change in both the form and the intensity of the interatomic interaction, with the accompaning restructuring of matter.

Atoms in the ground state are completely polarised in a strong magnetic field and therefore exhibit only weak interaction. Moreover, a gas of hydrogen-like atoms gives rise to a weakly nonideal Bose gas which does not solidify until zero temperature is reached. At the same time, weakly excited hydrogen atoms are able to form molecules with relatively high binding energy as well as long chains of polymeric molecules. The presence of hydrogen (or helium) molecules in the atmosphere of a pulsar can affect its cooling rate and is most likely to be detected in UV and x-ray spectra.

Estimates of the binding energy of matter at the neutron star's surface appear to confirm the validity of the magnetosphere models for free emission. Indeed, it has been shown that the binding energy of iron atoms is of the order of the surface temperature [25-27, 29], i.e. too low to interfere with free emission in strong electric fields.

However, an alternative scenario is conceivable, which has until now not been discussed in the literature. Hydrogen and helium accretion onto the surface of the pulsar can, in the course of time, result in the formation of molecules composed of alternating heavy and light atoms. Preliminary estimates suggest that the binding energy of such mixed molecules may be rather high. If more accurate calculations prove to support this conjecture, it will be possible to introduce the following new scenario of pulsar emission. Immediately after the birth of a pulsar, its magnetosphere is best described by the free-emission model. However, accumulation of light atoms on the stellar surface because of accretion eventually results in complete inhibition of the release of matter from the star (trapped emission). If pulsars are actually destined to develop along this line, freeemission models would be more appropriate to characterise younger stars, whereas trapped-emission models appear to be more suitable to describe older pulsars.

In conclusion, it seems appropriate to mention the novel mechanism of molecular laser radiation by hydrogen at the neutron star's surface. Such radiation is thought to originate from the transition between the strongly bound high-energy metastable state of hydrogen-like atoms in the singlet term and the practically unbound ground state of atoms. It is worthwile to note that the required pumping of the laser is provided by the reverse flow of high-energy particles, as stipulated by any model of the pulsar magnetosphere [22, 100].

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