

Matter in a Magnetic Field in the Thomas-Fermi and Related Theories

I. FUSHIKI

*Board of Studies in Astronomy and Astrophysics,
University of California at Santa Cruz, Santa Cruz, California 95064*

E. H. GUDDUNDSSON

Science Institute, University of Iceland, Dunhaga 3, IS-107 Reykjavik, Iceland

C. J. PETHICK

*Department of Physics, University of Illinois at Urbana-Champaign,
1110 W. Green Street, Urbana, Illinois 61801, and
Nordita, Blegdamsvej 17, DK-2100 Copenhagen Ø, Denmark*

AND

J. YNGVASON

Science Institute, University of Iceland, Dunhaga 3, IS-107 Reykjavik, Iceland

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We present a general discussion of the Thomas-Fermi (TF) and Thomas-Fermi-Dirac (TFD) approximations for the ground state properties of matter in a magnetic field taking all Landau levels into account. In the course of doing this we review some facts that are common to all theories of the TF type. Such theories are defined by specifying the energy density w of the electron gas as a function of the electron density n subject to some mild general requirements. Convexity of w is not needed, but singularities in ∇n occur if d^2w/dn^2 is not strictly positive. We also point out that the no binding theorem of TF theory holds irrespective of the shape of w . In TF theory with a magnetic field d^2w/dn^2 vanishes when new Landau bands begin to be populated and singular features in density profiles show up at such densities. These singularities are a rigorous consequence of quantum mechanics in the sense that TF theory becomes exact in the limit when the nuclear charges and the number of electrons tend to infinity, provided the magnetic field is scaled by the same factor as the charges to the power $\frac{1}{2}$. Apart from these features an atom with nuclear charge Z in a field of the order of $10^9 \times Z^{4/3}$ gauss exhibits a distinct shell structure associated with the Landau bands. The exchange energy of a homogeneous electron gas in a magnetic field is computed in a Hartree-Fock approximation. In particular we obtain closed expressions for the exchange energy for arbitrary Landau bands. The inclusion of the density of electrons in some Landau band changes discontinuously from zero to a finite value. A gradient correction (von Weizsäcker term) in the energy functional smooths out the discontinuities, but divergences in the density gradient reappear if the nuclear charges and the magnetic field tend to infinity as above. © 1992 Academic Press, Inc.

I. INTRODUCTION

The natural atomic unit for a magnetic field is $B^* = m_e^2 e^3 c / \hbar^3 = 2.35 \times 10^9$ gauss. Fields of this strength the Landau energy of an electron becomes comparable with the Rydberg energy, and the magnetic field has a decisive influence on the properties of matter. Although such high fields have not yet been produced in a terrestrial laboratory, they do occur in an astrophysical context, in particular at the surfaces of neutron stars, where fields are deduced to be as high as 10^{12} – 10^{13} gauss see, e.g., [1]). In laboratory semiconductors the characteristic field strength for the charge carriers may be considerably less than B^* , since carrier effective mass can be much smaller than the electron mass, and the Coulomb potential is dielectrically screened.

Theoretical studies of matter in high magnetic fields have been carried out using a variety of methods, see, e.g., [2–16]. Among these the Thomas–Fermi (TF) and Thomas–Fermi–Dirac (TFD) approximations used in [2–7] stand out as being particularly simple yet adequate for many purposes. Models of this type have been thoroughly studied in the past for the case of zero magnetic field [17–20]. In particular, the status of TF theory as an approximation to quantum mechanics was rigorously established in [18–21]: The theory is asymptotically exact in the limit when the nuclear charges and the number of electrons tend to infinity. This result can be generalized to the case where a magnetic field is present, provided the field strength is appropriately scaled together with the charges, cf. [22] and Section III below. Hence theories of TF type are expected to give a good picture of the ground state energy and the gross properties of a system of heavy nuclei and electrons. On the other hand, they are too crude to describe effects as delicate as molecular binding [18–20, 23].

In this paper we discuss various aspects of the TF and TFD approximations for the ground state of matter in a homogenous magnetic field, including a brief discussion of von Weizsäcker corrections to the energy functional. Previous treatments [2–7] have been concerned mainly with fields so strong that only the lowest Landau level is occupied. This is also the case in the papers [24, 25] that deal among other things with the extensions of the theory to non-zero temperatures. By contrast, as in [26] our emphasis is on effects that appear when more than one Landau level has to be taken into account. The basic aim is a qualitative understanding of these effects.

The paper is organized as follows. We begin, in Section II, with a summary of properties that are common to all theories of TF type. Applying an argument due to Benguria [27] we note that convexity of the energy density is not essential for the existence of a solution to the TF equation. On the other hand, a deviation from convex behavior will manifest itself as a singularity in the gradient of the electron density. We also point out that the no-binding theorem of TF theory is a very general result that does not depend on the detailed form of the energy density.

In Section III we consider the TF approximation without exchange for matter in a magnetic field. The kinetic energy density w_{kin} is a convex function of the electron

density n , but the second derivative $d^2 w_{\text{kin}} / dn^2$ vanishes where a new Landau band begins to be populated. This leads to a singularity of Vn at such densities. We discuss the scaling properties of TF theory with a magnetic field and the parameter range where the theory can be expected to be a valid approximation of the exact quantum-mechanical theory. In this section we also present the results of numerical TF calculations of the electronic densities of atoms in strong magnetic fields. Due to the scaling relations the profiles depend essentially only on the ratio $B/Z^{4/3}$, where B is the magnetic field strength and Z the nuclear charge. When this ratio is of the order 10^9 gauss, a TF atom shows a clear shell structure that is barely visible for much higher or much lower fields.

In Section IV we compute the energy density for a homogenous electron gas in a Hartree–Fock approximation including the exchange energy. This computation reveals a “swallowtail” instability in the neighborhood of the densities at which Landau bands begin to be occupied, and the energy density is no longer a convex function of the electron density. We then discuss qualitative features of TFD theory with a magnetic field. The non-convexity of the energy density leads in the TFD approximation to density jumps that are determined by a Maxwell construction. We estimate the size of these jumps for the case when the ratio between the magnetic length $l_B = (\hbar^2 / eB)^{1/2}$ and the Bohr radius a_0 may be regarded as a small parameter, and we find them to be of order $(l_B / a_0) \ln(a_0 / l_B)$, compared with the density steps determined by the Landau levels.

In Section V we consider the influence of the correction to the TFD energy functional of lowest order in the gradient of the electron density (von Weizsäcker term). This term involves the response function of the electron gas in a magnetic field. We do not attempt a detailed discussion of its form, but argue that it will smooth density profiles and effectively remove the jumps. The singular features of the TF approximation, however, are still present in the limit of high nuclear charges with an appropriately scaled magnetic field.

II. GENERAL FACTS ABOUT THOMAS–FERMI AND THOMAS–FERMI–DIRAC THEORIES

In this section we discuss some general properties that are common to all TF and TFD theories. Most of what we have to say is explicitly or implicitly contained in the (vast) literature on the subject, e.g., in Lieb’s comprehensive review article [20]. Nevertheless, we find it useful to collect these facts before we discuss the special case of matter in a magnetic field.

The TF method is the oldest and simplest case of a density functional theory (see, e.g., [28–30]). The total energy of a collection of electrons and nuclei is written as a functional $\mathcal{E}[n]$, where the density of electrons, $n = n(\mathbf{r})$, is a function of the position, \mathbf{r} . For a system having K nuclei with charges $Z_i e$ at fixed positions \mathbf{R}_i , $i = 1, \dots, K$, one assumes that \mathcal{E} has the form

$$\mathcal{E}[n] = \mathcal{E}_e[n] + \mathcal{V}_{ee}[n] + \mathcal{V}_{ez}[n] + \mathcal{Q}, \quad (2.1)$$

where the various terms are defined as follows. The n -independent term

$$q_0 = \sum_{i < j} \frac{e^2 Z_i Z_j}{|\mathbf{R}_i - \mathbf{R}_j|} \quad (2.2)$$

is the Coulomb interaction energy of the nuclei, and

$$\mathcal{V}_{eZ}[n] = -e \int n(\mathbf{r}) V(\mathbf{r}) d^3\mathbf{r} \quad (2.3)$$

with

$$V(\mathbf{r}) = \sum_i \frac{eZ_i}{|\mathbf{r} - \mathbf{R}_i|}, \quad (2.4)$$

the interaction energy between electrons and nuclei. The term

$$\mathcal{V}_{ee}[n] = \frac{e^2}{2} \iint \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3\mathbf{r} d^3\mathbf{r}' \quad (2.5)$$

represents the direct part of the Coulomb interaction between the electrons, and

$$\mathcal{E}[n] = \int w(n(\mathbf{r})) d^3\mathbf{r} \quad (2.6)$$

the kinetic part of the electronic energy (in TF theory), or the sum of the kinetic energy and the exchange energy (in TFD theory). In Thomas–Fermi–von Weizsäcker theory \mathcal{E}_e depends also on ∇n ; we shall consider that case in Section V.

The ground state energy of the system, E^{TF} , is given by the infimum of $\mathcal{E}[n]$ subject to the condition that $n \geq 0$ and that the total electronic charge is fixed:

$$\int n(\mathbf{r}) d^3\mathbf{r} = N. \quad (2.7)$$

For simplicity we shall in this paper almost exclusively consider neutral systems,

$$N = Z_1 + \dots + Z_K =: Z. \quad (2.8)$$

Generalizations to positive ions, $N < Z$, are straightforward, but occasionally they make the discussion slightly more cumbersome. Negative ions, $N > Z$, do not exist in TF theory (cf [20, Theorem 2.5]).

A minimizing density n for (2.1) solves the TF equation

$$w'(n(\mathbf{r})) - e\phi(\mathbf{r}) - \mu_{\text{tot}} \begin{cases} = 0 & \text{if } n(\mathbf{r}) > 0 \\ \geq 0 & \text{if } n(\mathbf{r}) = 0, \end{cases} \quad (2.9)$$

where the prime denotes differentiation with respect to n ,

$$\phi(\mathbf{r}) = V(\mathbf{r}) - e \int \frac{n(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3\mathbf{r}' \quad (2.10)$$

is the total electrostatic potential, and the Lagrange multiplier μ_{tot} is determined by condition (2.7). Conversely, a solution of (2.9) minimizes \mathcal{E} with the subsidiary condition (2.7), where N is uniquely determined by μ_{tot} . For $n(\mathbf{r}) > 0$, Eq. (2.9) can be written

$$\mu_{\text{tot}} = \frac{\delta \mathcal{E}[n]}{\delta n(\mathbf{r})} = \frac{dE^{\text{TF}}}{dN}, \quad (2.11)$$

so its physical meaning is that the total electrochemical potential of an electron is everywhere equal to the constant μ_{tot} .

The following conditions on w guarantee the existence and uniqueness of a solution to (2.9) and (2.7) for $N \leq Z$ (apply Theorem 3.18 in Lieb [20] with $j(n) = w(n) - w'(0)n$):

- (i) $w(0) = 0$, w is continuously differentiable and convex.
- (ii) For large n , $w'(n) \geq c \cdot n^{1/2+\epsilon}$ with c and $\epsilon > 0$.
- (iii) For small n , $w'(n) \leq c'n^{1/3+\epsilon}$, $c' < \infty$, $\epsilon > 0$.

We now comment on these conditions. If (ii) is not satisfied, $\mathcal{E}[n]$ need not be bounded below: If $w(n) = \text{const} \cdot n^{3/2}$ and $n(\mathbf{r})$ behaves like $|\mathbf{r} - \mathbf{R}_i|^{-(2-\epsilon)}$ in a neighborhood of the nuclei, then $\mathcal{E}[n] \rightarrow -\infty$ for $\epsilon \rightarrow 0$. This corresponds physically to the pressure of the electron gas being insufficient to prevent atoms from collapsing. If (iii) is not satisfied, then (2.9) need not have a solution satisfying (2.7) for all $N \leq Z$. The reason is that if $w'(n)$ is too large at low densities it pays energetically to reduce the electron density by pushing part of the charge towards infinity. The infimum of \mathcal{E} over all n with a given total charge then is not a minimum.

As for condition (i), we remark that convexity of w seems at first to be an essential ingredient of the existence proof, which uses techniques from nonlinear functional analysis [19, 20]. However, as we shall see below, this assumption is in fact superfluous because the theory automatically “corrects” any deviation from convex behavior of w . Before discussing this in more detail we comment on the physical significance of this convexity.

If $v = n^{-1}$ denotes the specific volume of the electron gas, then $\mathcal{W} = v \cdot w$ is the specific kinetic (plus exchange) energy, and

$$P_{\text{loc}} = -\frac{d\mathcal{W}(v)}{dv} = w'(n)n - w(n) \quad (2.12)$$

can be interpreted as the local electronic pressure. Indeed, it follows from the TF equation (2.9) that

$$\nabla P_{\text{loc}} = en \nabla \phi, \quad (2.13)$$

which is precisely the condition for hydrostatic equilibrium between the Coulomb forces and the pressure gradient. If w is convex and $w(0) = 0$, then obviously

$$P_{\text{loc}} \geq 0. \quad (2.14)$$

The compressibility κ of the electron gas is given by

$$\kappa^{-1} = -v \frac{dP_{\text{loc}}}{dv} = n^2 w''(n). \quad (2.15)$$

Hence convexity of w is equivalent to $\kappa \geq 0$. We also note that P_{loc} is the Legendre transform of w , so P_{loc} is a convex function of $\mu = w'$ if w is convex.

Suppose now that w is not convex in some density interval, i.e., that $w''(n) = 0$ for $n^{(1)} < n < n^{(2)}$, say (see Fig. 1). We claim that the solution of the TF equation (2.9) does not take on values in this interval. In fact, suppose $n^{(1)} < n(\mathbf{r}) < n^{(2)}$ for all \mathbf{r} in some region. By (2.9) we then have $\nabla^2 \phi(\mathbf{r}) = 0$ for these \mathbf{r} . But this contradicts $\nabla^2 \phi(\mathbf{r}) = 4\pi e [n(\mathbf{r}) - \sum_i Z_i \delta(\mathbf{r} - \mathbf{R}_i)]$ which follows from (2.10). (This remark is due to Benguria [27], cf. Lieb [20, Theorem 3.19]. Note that it applies also if the positive charge has a continuous distribution, as long as the positive charge density avoids intervals where w is not strictly convex.)

The argument above can also be stated in terms of the compressibility and pressure of the electron gas as follows:

If $w''(n)$ vanishes for some n , then the compressibility diverges at this density. This can be interpreted as a phase transition with the densities $n^{(1)}$ and $n^{(2)}$ at the end points of the interval with $w'' = 0$ corresponding to pure phases. In fact, the electronic chemical potential, given by

$$\mu(n) = w'(n) = \mu_{\text{ion}} + e\phi, \quad (2.16)$$

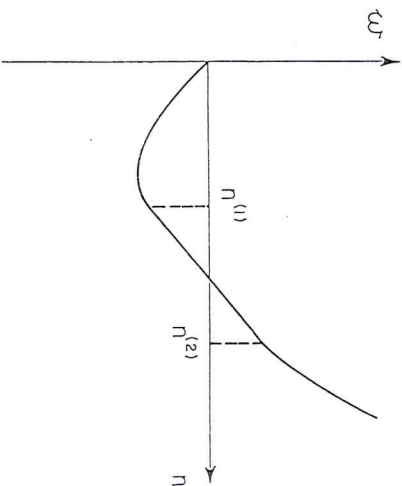


FIG. 1. An example of a convex energy density, w , with $w'' = 0$ for $n^{(1)} < n < n^{(2)}$. The solution of the TF equation does not take values in the interval $(n^{(1)}, n^{(2)})$.

and the pressure (2.13) satisfy the equilibrium conditions

$$\mu(n^{(1)}) = \mu(n^{(2)}) \quad (2.17)$$

and

$$P_{\text{loc}}(n^{(1)}) = P_{\text{loc}}(n^{(2)}). \quad (2.18)$$

Because the compressibility diverges for n between $n^{(1)}$ and $n^{(2)}$, it is clear that mixtures of the two phases (with intermediate densities between $n^{(1)}$ and $n^{(2)}$) can be stable only in regions where the pressure is constant. But if $\nabla P_{\text{loc}}(\mathbf{r}) = 0$, then $\nabla^2 \phi(\mathbf{r}) = 0$ by (2.13). This is impossible for nonvanishing densities because ϕ has to satisfy the Poisson equation $\nabla^2 \phi(\mathbf{r}) = 4\pi e [n(\mathbf{r}) - \sum_i Z_i \delta(\mathbf{r} - \mathbf{R}_i)]$.

The observation that the solution of (2.9) avoids flat portions of the graph of w' leads to an interesting generalization of the results considered so far:

A unique solution to the TF problem, i.e., of Eqs. (2.9) and (2.7), exists for any energy density, w , with the property that its *convex hull*

$$w^*(n) = \sup \{l(n) \mid l(n') = a \cdot n' + b, l(n') \leq w(n')\} \quad (2.19)$$

satisfies conditions (i)-(iii) stated above. Moreover, this solution is *identical* to the solution with w replaced by w^* .

To prove this claim (cf. Theorem 6.8 in Lieb [20]), we note that $w^* \leq w$, so $\mathcal{E}^*[n] \leq \mathcal{E}[n]$, where \mathcal{E}^* denotes the functional (2.1) with w replaced by w^* . Hence $\inf \mathcal{E}^*[n] \leq \inf \mathcal{E}[n]$. On the other hand, if n^* denotes the (unique) density with $\inf \mathcal{E}^*[n] = \mathcal{E}^*[n^*]$, we have $\mathcal{E}[n^*] = \mathcal{E}^*[n^*]$, because n^* omits the values where w and w^* differ. Thus, $\mathcal{E}[n^*] = \mathcal{E}^*[n^*] = \inf \mathcal{E}^*[n] \leq \inf \mathcal{E}[n]$, so n^* is a minimizing density for \mathcal{E} . This density is unique because $n \neq n^*$ implies $\mathcal{E}[n^*] = \mathcal{E}^*[n^*] < \mathcal{E}^*[n] \leq \mathcal{E}[n]$.

Figure 2 illustrates the points discussed above. Note that although $w'' \geq 0$ on

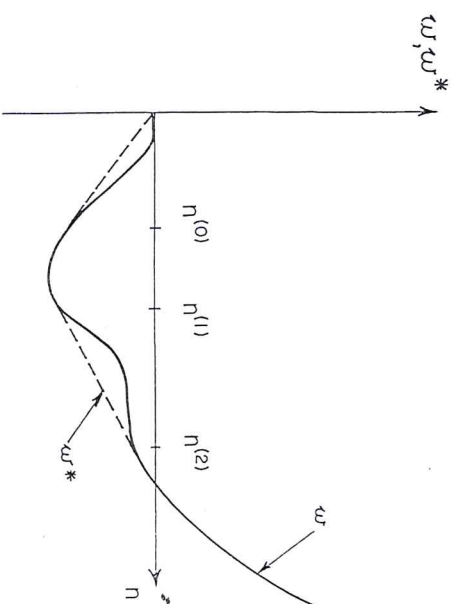


FIG. 2. An example of an energy density, w , with its convex hull, w^* . The TF equation has no solutions with densities less than $n^{(0)}$ or in the interval $(n^{(1)}, n^{(2)})$.

parts of the interval between $n^{(1)}$ and $n^{(2)}$, these densities are also excluded. The same applies to the interval $(0, n^{(0)})$ in Fig. 2; here we note that for densities below $n^{(0)}$ the pressure would be negative. The density $n^{(0)}$ is a minimal density > 0 for the TF theory corresponding to an energy density w of this shape. It is determined by the condition

$$P_{\text{loc}}(n^{(0)}) = w'(n^{(0)})n^{(0)} - w(n^{(0)}) = 0. \quad (2.20)$$

Since n must tend to zero at infinity, it is clear that a system with such a minimal density $n^{(0)} > 0$ has a finite spatial extent with the density dropping abruptly to zero at the boundary. A calculation for a single atom with a w of the shape shown in Fig. 2 would show a density profile as pictured in Fig. 3a; the corresponding Φ and P_{loc} are shown schematically in Figs. 3b and 3c.

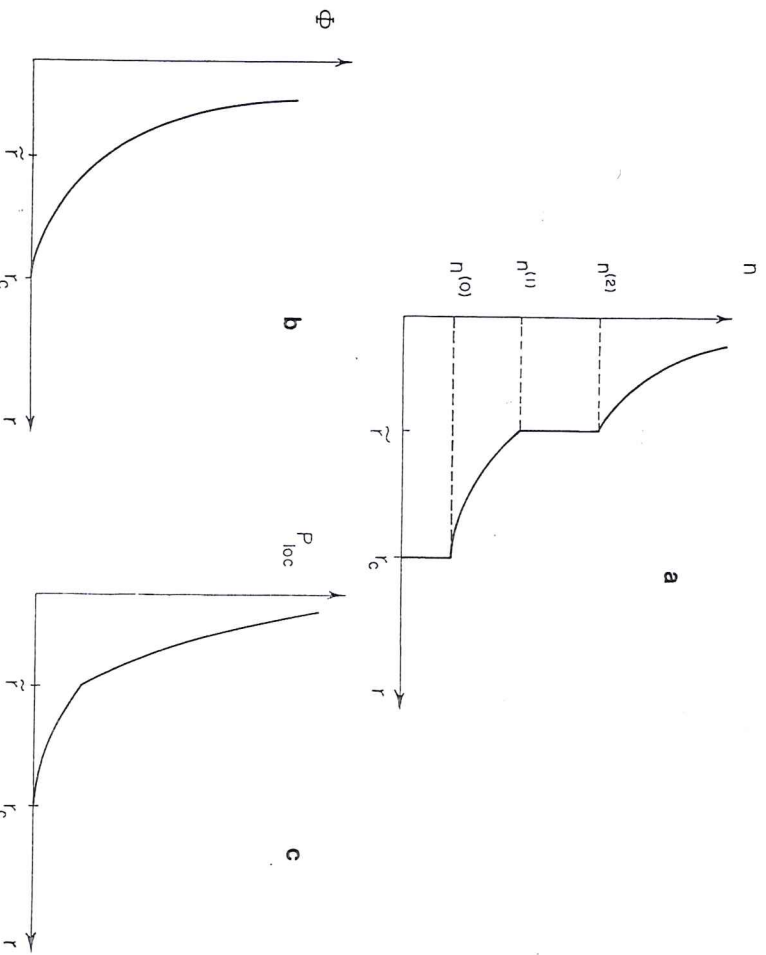


Fig. 3. The figure shows in a schematic way the results of a typical TFD calculation for an isolated atom with the energy function shown in Fig. 2: (a) The density profile. The electron density, n , decreases monotonically from ∞ at the nucleus to $n^{(0)}$ at $r = r_c$ (edge of the atom). At $r = \tilde{r}$ there is a jump in the density from $n^{(2)}$ to $n^{(1)}$. At the edge $dn/dr = 0$. (b) The electrostatic potential, Φ . This behaves as $Z\phi/r$ for small r and decreases monotonically to 0 at $r = r_c$. The potential is continuous everywhere (also at $r = \tilde{r}$) and vanishes at the edge. (c) The local pressure, P_{loc} , diverges for small r and decreases to 0 at the edge. dP/dr also vanishes at the edge and is discontinuous at $r = \tilde{r}$.

Isolated zeros of w'' for an otherwise convex energy density will also lead to singular behaviour of the electron density. In fact, by the TF equation (2.9) we have

$$\nabla n(\mathbf{r}) = e \nabla \Phi(\mathbf{r})/w''(n(\mathbf{r})). \quad (2.21)$$

Hence the density gradient diverges if w'' approaches zero. As we shall see in Section III this situation occurs in the TF approximation for matter in a magnetic field, leading to a density profile of the type shown in Fig. 6.

The last subject we discuss in this section is the absence of molecular binding in theories of the TF type. About 35 years ago Sheldon [31] discovered by a numerical calculation that the N_2 molecule has no stable equilibrium in the TFD approximation. This was explained several years later when Teller [23] proved the so-called "no-binding theorem" for the TF and TFD theories. Subsequently the problem was investigated in a more rigorous fashion and extended by Lieb and Simon [18, 19], Benguria [27], and Lieb [20].

The no-binding theorem can be stated in the following way: Consider a collection of nuclei fixed in space surrounded by electrons. Then the TF approximation for the energy of the collection will always decrease if the nuclei are separated into two or more groups which are moved far away from each other, i.e., $E \geq E_1 + E_2 + \dots$, where the E_j are the TF energies of the individual subgroups and E is the original TF energy of the collection. This means, in particular, that in TF theory any molecule is unstable under decomposition into isolated atoms. The no-binding theorem clearly demonstrates the approximate nature of the TF method, since real atoms do bind to form molecules.

In his original paper Teller investigated molecular binding in matter with the energy density w used in standard TF and TFD theories for zero magnetic field:

$$w(n) = w_{\text{kin}}(n) = \{3(3\pi^2)^{2/3} \hbar^2 / (10m)\} n^{5/3} \quad (2.22)$$

for TF theory, with m the electron mass, and

$$w(n) = w_{\text{kin}}(n) + w_{\text{ex}}(n) \quad (2.23)$$

with

$$w_{\text{ex}}(n) = -(4/3)(3/\pi)^{1/3} e^{-2} n^{4/3} \quad (2.24)$$

for TFD theory.

The papers by Lieb, Simon, and Benguria are also concerned mainly with these special forms of w . However, their extension of Teller's work is in fact quite general, and it follows from Theorem 3.23 in Lieb [20] that binding does not occur for any w satisfying conditions (i)-(iii) in the previous section. This is also obvious from the proof given in Lieb [32] for $w(n) = \text{const} \cdot n^{5/3}$. Granted the existence of a solution for (2.9), the only special property of this function, that is used, is its convexity. But, as discussed above, the TF energies calculated with an arbitrary w are the same as those calculated with its convex hull, w^* . Thus the no-binding theorem

olds for any w , provided its convex hull satisfies conditions (i)–(iii) above so that the TF approximation is well defined. The energy density for matter in a magnetic field that is discussed in the next sections fulfills these requirements.

Closely related to the no-binding theorem is the positivity of the global pressure. A finite system with nuclei in arbitrary positions, there are various ways of finding the global pressure, but the following is perhaps the most natural one [20, 33]: One considers a uniform dilation of the system, such that the nuclei move from \mathbf{R}_i to $a\mathbf{R}_i$. The TF energy E^{TF} of the system then becomes a function of a , and one defines

$$P_{\text{glob}} = -\frac{dE^{\text{TF}}}{d(a^3)} = -\frac{1}{3a^2} \frac{dE^{\text{TF}}}{da}. \quad (2.25)$$

Positivity of the global pressure means that the system is unstable with respect to local dilations, not only under the global dilation $a \rightarrow \infty$, as claimed by the no-binding theorem. When the nuclei are arranged in a regular lattice, one can think of a as measuring the size of the unit cell. In the Wigner–Seitz approximation, where the unit cell is approximated by a sphere, (2.25) is precisely the definition of pressure used in Fushiki *et al.* [7]. As shown in Appendix B of that paper, his pressure is equal to the local pressure (2.12) at the boundary of the spheres. According to the discussion in the previous section, the local pressure is always ≥ 0 , so the same holds for the global pressure in this approximation.

A general proof of the positivity of (2.25) is, of course, more difficult. It has been carried out by Benguria and Lieb [33] for the standard TF theory with w as in (2.22). Although we expect that it also holds for general w under the same conditions as the no-binding theorem, it is not known to us whether the proof of Lieb and Benguria can be extended to cover this case.

III. THOMAS–FERMI THEORY FOR MATTER IN A MAGNETIC FIELD

In this section we recall the basic properties of the uniform electron gas in a magnetic field in the absence of electron–electron interactions and investigate qualitative features of TF theory with the corresponding energy density. We also consider the scaling properties of TF theory and discuss its expected range of validity.

The energy levels of a non-relativistic free electron in a homogenous magnetic field \mathbf{B} are given by

$$\epsilon_{p\alpha\sigma}^0 = \left(\alpha + \frac{1}{2} + \sigma \right) \hbar\omega_B + \frac{p^2}{2m}, \quad (3.1)$$

where α is a non-negative integer specifying the Landau band, σ is the spin component and p is the momentum component along the field, m is the electron mass, and

$\omega_B = eB/(mc)$ is the cyclotron frequency (see, e.g., Landau and Lifshitz [34]). In addition, there is a degeneracy that can be indexed, e.g., by the orbital angular momentum M along the field; the number of states per unit area is $(2\pi l_B^2)^{-1}$ with $l_B = (\hbar c/(eB))^{1/2}$ the magnetic length, that is, one state for every quantum of flux hc/e .

We note that the magnetic length can be written as $l_B = a_0(B/B^*)^{-1/2}$, where $a_0 = \hbar^2/(me^2) = 0.529 \times 10^{-8}$ cm is the Bohr radius and $B^* = m^2 e^3 c/\hbar^3 = 2.35 \times 10^9$ gauss is the natural atomic unit for the magnetic field. In terms of $B_{12} := B[\text{gauss}]/10^{12}$ one has, therefore, $l_B = 2.57 \times 10^{-10} B_{12}^{-1/2}$ cm, or $a_0/l_B = 20.7 B_{12}^{1/2}$.

If one chooses the vector potential to be $\mathbf{B} \times \mathbf{r}/2$ (symmetric gauge), and uses cylindrical coordinates ρ, z, ϕ , with the z -axis in the direction of the field, one may write the wavefunctions as

$$\psi_{p\alpha\sigma M}(\rho, z, \phi) = \frac{1}{\sqrt{2\pi l_B^2 L}} \left[\frac{\alpha'!}{(|M| + \alpha')!} \right]^{1/2} \times e^{i(pz/\hbar + eM\phi/\hbar)} |M| e^{-\eta^2/2} L_{|M|}^{\alpha'}(\eta^2) \chi_{\sigma}, \quad (3.2)$$

cf. [34]. Here L is the normalization length in the direction of the field, $\eta = \rho/\sqrt{2} l_B$, L_{α}^{β} are associated Laguerre polynomials (normalized as in [35, p. 775]), and χ_{σ} is the spin- $\frac{1}{2}$ wavefunction. The angular momentum M takes integer values from α down to $-\infty$, and $\alpha' = \alpha$ for $M \leq 0$, $\alpha' = \alpha - M$ for $M = 1, \dots, \alpha$. For the lowest Landau band, $\alpha = 0$, the wavefunction $\psi_{p\alpha\sigma M}$ is proportional to $e^{iM\phi} \rho^{|M|} e^{-\rho^2/4l_B^2} e^{ipz/\hbar} \chi_{\sigma}$. Since the single-electron energies do not depend on M , the occupation number, $f_{p\alpha\sigma}$, is in thermal equilibrium independent of M .

Let $n_{p\alpha\sigma}$ denote the density of electrons with given values of p, α , and σ but arbitrary values of M . We have

$$n_{p\alpha\sigma} = f_{p\alpha\sigma} / (2\pi l_B^2 L) \quad (3.3)$$

and the energy density is

$$w = \sum_{p\alpha\sigma} \epsilon_{p\alpha\sigma}^0 n_{p\alpha\sigma}, \quad (3.4)$$

where in the ground state the sum is over the lowest energy levels for a given total electron density

$$n = \sum_{p\alpha\sigma} n_{p\alpha\sigma}. \quad (3.5)$$

The Fermi momentum of a band $\alpha\sigma$ is

$$p_{F\alpha\sigma} = \{ 2m(\mu - (\alpha + \sigma + \frac{1}{2})\hbar\omega_B) \}^{1/2} \theta(\mu - (\alpha + \sigma + \frac{1}{2})\hbar\omega_B), \quad (3.6)$$

where $\mu = dW/dn$ is the chemical potential (Fermi energy) and θ denotes the

Heaviside step function. The particle density in the band is $n_{\alpha\sigma} = \sum_{\rho} n_{\rho\alpha\sigma}$, and, replacing \sum_{ρ} by $L \int_{-d\rho}^{d\rho} d\rho / (2\pi\hbar)$, we obtain

$$n_{\alpha\sigma} = \frac{P_{F\alpha\sigma}}{2(\pi l_B)^2 \hbar}. \quad (3.7)$$

Since the single particle energy depends on α and σ in the combination $\nu = (\alpha + \sigma + \frac{1}{2})$, we may replace the sum over α and σ by one over non-negative integers ν . The states with $\nu = 0$ are singly degenerate, corresponding to $\alpha = 0$ and $\sigma = -\frac{1}{2}$, while those for $\nu > 0$ are doubly degenerate, corresponding to $\alpha = \nu$, $\sigma = -\frac{1}{2}$ and $\alpha = \nu - 1$, $\sigma = \frac{1}{2}$. If one introduces the dimensionless variable $\zeta := \mu / (\hbar\omega_B)$ one may write $n = \sum_{\nu} n_{\nu}$ as

$$n = n_* \left[\zeta^{1/2} + 2 \sum_{\nu=1}^{[\zeta]} (\zeta - \nu)^{1/2} \right], \quad (3.8)$$

where

$$n_* := \frac{2}{\pi^{1/2}} \left(\frac{eB}{\hbar c} \right)^{3/2} \frac{1}{2^{1/2} \pi^2} \cdot l_B^{-3} = 4.24 \times 10^{27} B_{12}^{3/2} \text{ cm}^{-3} \quad (3.9)$$

and $[\zeta]$ denotes the integer part of ζ . In the same way we obtain for the energy (3.4)

$$w = \frac{1}{3} n_* \hbar\omega_B \left[\zeta^{3/2} + 2 \sum_{\nu=1}^{[\zeta]} (\zeta + 2\nu)(\zeta - \nu)^{1/2} \right]. \quad (3.10)$$

The density at which the ν th band begins to be populated, i.e., for which $\zeta = \nu$, is by (3.8)

$$n_*^{(\nu)} = n_* \left[\nu^{1/2} + 2 \sum_{\nu'=1}^{\nu-1} (\nu - \nu')^{1/2} \right]. \quad (3.11)$$

From (3.11) one finds

$$(n_*^{(\nu+1)} - n_*^{(\nu)}) / n_* = \nu^{1/2} + (\nu + 1)^{1/2} \quad (3.12)$$

and thus

$$n_*^{(\nu)} \approx (4/3) n_* \nu^{3/2} \quad (3.13)$$

for large ν . As was to be expected this result agrees with that for a three-dimensional Fermi gas in zero magnetic field, $n = P_F^3 / (3\pi^2 \hbar^3)$, for $P_F = (2m\mu)^{1/2}$.

From (3.8) it follows that just above $n_*^{(\nu)}$,

$$\mu(n) = \hbar\omega_B \left[\nu + \frac{c_{\nu}}{n_*} (n - n_*^{(\nu)})^2 + O(|n - n_*^{(\nu)}|^3) \right] \quad (3.14)$$

and

$$w(n) = w(n_*^{(\nu)}) + \hbar\omega_B \left[\nu \cdot (n - n_*^{(\nu)}) + \frac{c_{\nu}}{3n_*} (n - n_*^{(\nu)})^3 + O(|n - n_*^{(\nu)}|^4) \right] \quad (3.15)$$

with $c_0 = 1$ and $c_{\nu} = \frac{1}{4}$ for $\nu \geq 1$. In particular, the second derivative $d^2 w / dn^2 = d\mu / dn$ vanishes if n tends towards $n_*^{(\nu)}$ from above. On the other hand, for $n \neq n_*^{(\nu)}$ one has by (3.10)

$$\frac{d^2 w}{dn^2} = \frac{2\hbar\omega_B}{n_*} \left[\zeta^{-1/2} + 2 \sum_{\nu=1}^{[\zeta]} (\zeta - \nu)^{-1/2} \right]^{-1}, \quad (3.16)$$

and if n tends towards $n_*^{(\nu)}$ from below one obtains

$$w''(n_*^{(\nu)-}) = \frac{2\hbar\omega_B}{n_*} \left[\nu^{-1/2} + 2 \sum_{\nu'=1}^{\nu-1} (\nu - \nu')^{-1/2} \right]^{-1}. \quad (3.17)$$

Thus $d^2 w / dn^2$ is discontinuous at $n = n_*^{(\nu)}$. For large ν (3.17) can be approximated as

$$w''(n_*^{(\nu)-}) \approx \frac{\hbar\omega_B}{2n_*} \nu^{-1/2} \approx \frac{\hbar^2}{m} \left(\frac{\pi^4}{3} \right) n_*^{(\nu)-1/3}, \quad (3.18)$$

cf. the zero field case (2.22). Plots of $w(n)$, $\mu(n)$, and $w''(n)$ are shown in Fig. 4.

Next we discuss the scaling properties of TF theory for matter in a magnetic field. Inverting (3.8) we can write

$$\mu = \hbar\omega_B \tilde{\mu}(n/n_*) = Bf(n/B^{3/2}) \quad (3.19)$$

and, hence,

$$w = \hbar\omega_B n_* \tilde{w}(n/n_*) = B^{5/2} F(n/B^{3/2}). \quad (3.20)$$

From this it follows that the TF equation (2.9), which for $w' \geq 0$ may be written as

$$w'(n(\mathbf{r})) = [e\Phi(\mathbf{r}) + \mu_{\text{tot}}]_+, \quad (3.21)$$

and the normalization condition $\int nd^3\mathbf{r} = \sum_i Z_i$ are invariant under the following substitutions:

$$\begin{aligned} Z_i &\rightarrow aZ_i, \\ B &\rightarrow a^{4/3} B, \\ \mathbf{R}_i &\rightarrow a^{-1/3} \mathbf{R}_i, \\ \mu_{\text{tot}} &\rightarrow a^{4/3} \mu_{\text{tot}}, \\ n(\mathbf{r}) &\rightarrow a^2 n(a^{1/3} \mathbf{r}) =: n_a(\mathbf{r}). \end{aligned} \quad (3.22)$$

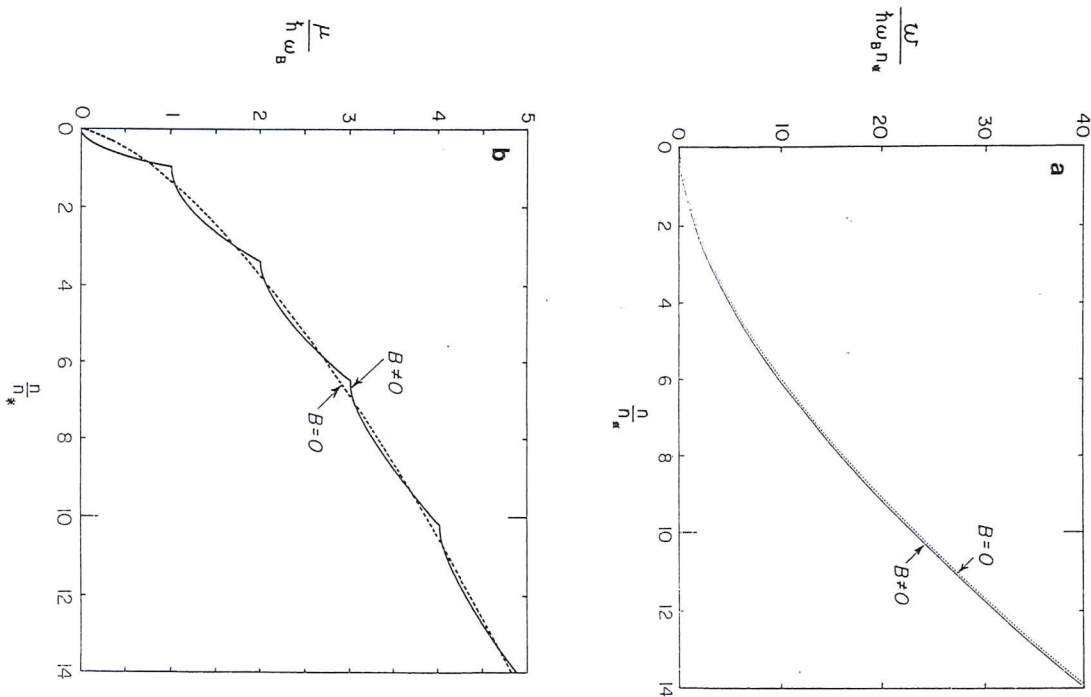


Fig. 4. (a) The energy density, $w(n)$, of the homogeneous electron gas in a magnetic field without the exchange contribution. The dashed line shows the result corresponding to matter in zero field, which may be written as $w = (1/10)(3^5/2)^{1/3} n^* \hbar \omega_B (n/n_*)^{5/3}$. (b) The chemical potential, $\mu(n) = w'(n)$, corresponding to the energy density in (a). The dashed line shows the zero field result. (c) The second derivative of w with respect to n , $w''(n)$, for the energy density in (a). The dashed line shows the zero field result.

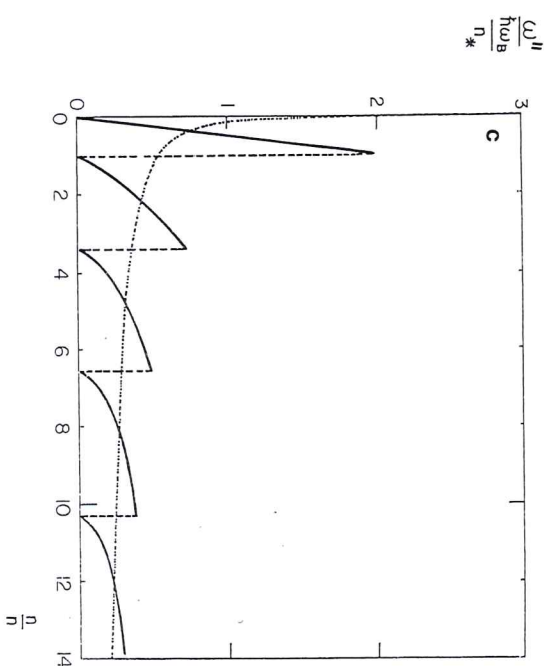


Figure 4—Continued

Moreover, the energy functional (2.1) has the scaling property

$$\mathcal{E}[n_a; aZ, a^{4/3}B, a^{-1/3}\mathbf{R}_i] = a^{7/3} \mathcal{E}[n; Z, B, \mathbf{R}_i] \quad (3.23)$$

and the TF energy, $E^{\text{TF}} = \inf\{\mathcal{E}[n] | \int n d^3\mathbf{r} = \sum_i Z_i\}$, transforms accordingly:

$$E^{\text{TF}}(aZ, a^{4/3}B, a^{-1/3}\mathbf{R}_i) = a^{7/3} E^{\text{TF}}(Z, B, \mathbf{R}_i). \quad (3.24)$$

A notable feature of the scaling relations (3.22) is that the inter-electron spacing and the magnetic length both scale as $a^{-2/3}$. It is this fact that makes the electron energy scale simply. One consequence of the scaling laws is that the shape of an atom in TF theory depends only on B and Z in the (dimensionless) combination

$$\beta := \frac{B/B_*}{Z^{4/3}}. \quad (3.25)$$

More precisely, in a plot of n/Z^2 (or of n/n_*) as a function of $Z^{1/3}|\mathbf{r}|$, all atoms look the same for fixed β . The charge distribution for different values of β is shown in Fig. 5. For *weak fields*, i.e., $\beta \ll 1$, as well as *strong fields*, i.e., $\beta \gg 1$, the density profiles look smooth; for β of order 1, however, they have clearly discernable features associated with the occupation of new Landau bands. These features are shown in a closeup in Fig. 6. In Fig. 7 the radial density $r^2 n(r)$ is plotted for an iron atom ($Z=26$) and field strength $B=10^{11}$ and 10^{12} gauss. The corresponding values of β are 0.55 and 5.55. The shell structure due to the magnetic field is particularly distinct in the former case.

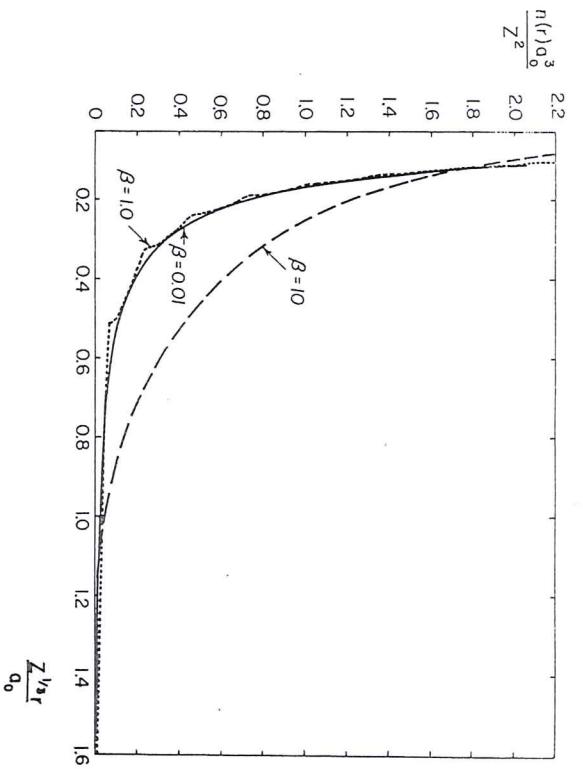


Fig. 5. The charge distribution in an atom in a magnetic field as calculated by the TF method for several values of $\beta = (B/B^*)/Z^{4/3}$.

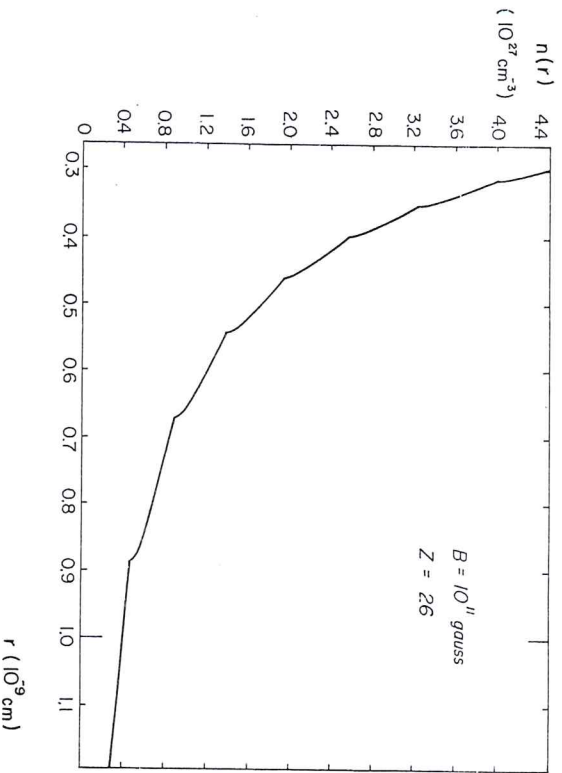


Fig. 6. Close-up of the singular features of an atomic density for $\beta = 0.55$.

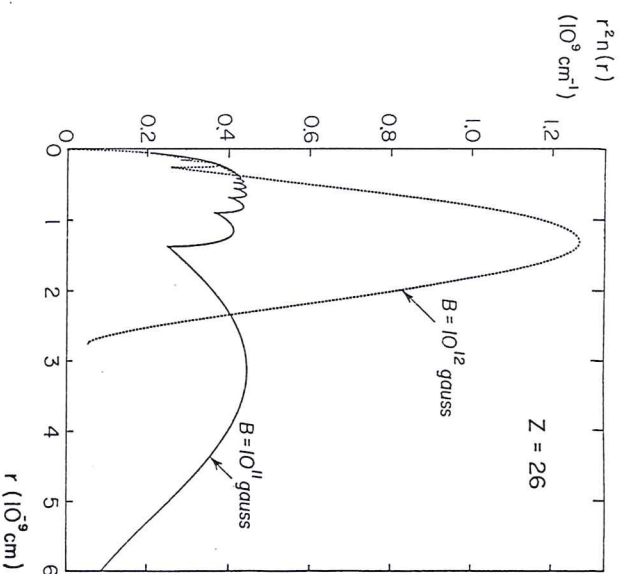


Fig. 7. A plot of $r^2 n(r)$ as a function of r in TF theory for an iron atom ($Z=26$) in a magnetic of $B=10^{11}$ and $B=10^{12}$ gauss. The corresponding values of β are 0.55 and 5.5.

A qualitative understanding of these profiles is easily obtained by solving (2.21) for densities just above $n_*^{(v)}$ with the approximations $\nabla\Phi \sim eZ/(Z^{-1/3}a_0)^2 \sim Z^{5/3}$ and $w'' \sim B^{-2}(n - n_*^{(v)})$. If $r^{(v)}$ denotes the radius at which $n = n_*^{(v)}$ one finds

$$(n - n_*^{(v)}) \sim BZ^{5/6}(r^{(v)} - r)^{1/2}, \quad (3.26a)$$

or, equivalently,

$$(n - n_*^{(v)})/Z^2 \sim \beta(Z^{1/3}(r^{(v)} - r))^{1/2}, \quad (3.26b)$$

as r approaches $r^{(v)}$ from below. On the other hand, $n(r)$ has a finite slope if r approaches $r^{(v)}$ from above, by (2.21) and (3.17). It should be noted that singularities in the density gradient are present at all values of β . From (3.26b) and the fact that $(n_*^{(v+1)} - n_*^{(v)})/Z^2 \sim \beta^{3/2}$ (3.12), one can see that these features become invisible as $\beta \rightarrow 0$, however. For $\beta \gg 1$ the singularities occur only very close to the nuclei, where the density gradient is high anyway.

In the strong field regime, $\beta \gg 1$, we can approximate $w(n)$ at the relevant densities by $\frac{1}{2}\hbar\omega_B n^3/n_*^2 \sim n^3/B^2$. In this regime the theory is approximately invariant under additional scaling transformations for fixed Z , [5]:

$$\begin{aligned} B &\rightarrow bB, \\ \mathbf{R}_i &\rightarrow b^{-2/5}\mathbf{R}_i, \end{aligned} \quad (3.27)$$

$$n(\mathbf{r}) \rightarrow b^{6/5}n(b^{2/5}\mathbf{r}),$$

with

$$E^{\text{TF}} \rightarrow \beta^{2/5} E^{\text{TF}}. \quad (3.28)$$

From (3.27) and (3.22) it follows that for $\beta \gg 1$ the radius of an atom is proportional to $Z^{1/5}/B^{2/5}$. In a plot as above, Fig. 5, the radius of an atom thus shrinks as $\beta^{-2/5}$ for $\beta \rightarrow \infty$.

As mentioned in the Introduction it can be rigorously proved that TF theory with a homogeneous magnetic field is a scaling limit of quantum mechanics. For zero magnetic field this was shown by Lieb and Simon [18, 19] and Baumgartner [21], cf. also Lieb [20, section V]. The proof given in [20] was extended to the case of a homogeneous field in [22], making use of the B -independent lower bound for the kinetic energy established in [36]. The precise assertion is as follows:

Let $E^{\text{QM}}(Z_i, B, \mathbf{R}_i)$ denote the exact quantum mechanical ground state energy and $n^{\text{QM}}(r; Z_i, B, \mathbf{R}_i)$ denote the corresponding electronic density (assuming here for simplicity that there is a unique ground state). Then

$$\lim_{a \rightarrow \infty} E^{\text{QM}}(aZ_i, a^{4/3}B, a^{-1/3}\mathbf{R}_i)/a^{7/3} = E^{\text{TF}}(Z_i, B, \mathbf{R}_i) \quad (3.29)$$

and

$$\lim_{a \rightarrow \infty} n^{\text{QM}}(a^{-1/3}\mathbf{r}; aZ_i, a^{4/3}B, a^{-1/3}\mathbf{R}_i)/a^2 = n^{\text{TF}}(\mathbf{r}; Z_i, B, \mathbf{R}_i), \quad (3.30)$$

the convergence of n^{QM} to the TF density n^{TF} being in the weak L_1 sense.

Note that the way in which quantum mechanics passes over into TF theory is dictated by the scaling properties (3.22) and (3.23) of the latter. As a supplement to the rigorous proof in [22] we shall below try to make the limit theorems plausible by comparing the various length scales of the problem. At the same time one obtains some insight into the parameter range where the approximation may be expected to be good. For the case of strong fields similar discussions may be found in [3-5].

The basic lengths for an atom are the Bohr radius $a_0 = \hbar^2/(me^2)$ and the magnetic length $l_B = (\hbar c/eB)^{1/2}$. The strong field case,

$$B^* Z^{4/3} < B, \quad (3.31)$$

corresponds to $l_B < Z^{-2/3}a_0$ and the weak field case,

$$B < B^* Z^{4/3}, \quad (3.32)$$

to $l_B > Z^{-2/3}a_0$; the length $Z^{-2/3}a_0$ can be regarded as the mean electronic separation in zero field. Let \bar{r} denote the mean radius of the charge distribution. The Fermi wavelength λ_F at electronic densities of order Z/\bar{r}^3 is $\lambda_F \sim \bar{r}/Z^{1/3}$ in the weak field case and $\lambda_F \sim \bar{r}^3/(Zl_B^2)$ for strong fields. We estimate \bar{r} by equating the kinetic energy $\sim \hbar^2/(m\lambda_F^2)$ and the Coulomb energy of an electron, Ze^2/\bar{r} . This gives

$$\bar{r} \sim Z^{-1/3}a_0 \quad (3.33)$$

for weak fields and

$$\bar{r} \sim (Za_0 l_B^2)^{1/5} = \beta^{-2/5} Z^{-1/3} a_0 \quad (3.34)$$

for strong fields. We expect TF theory to be a reasonable approximation if $\lambda_F \ll \bar{r}$. This is equivalent to the conditions

$$1 \ll Z^{1/3} \quad (3.35)$$

for weak fields and

$$B \ll B^* Z^3 \quad (3.36)$$

for strong fields. A Z - B diagram indicating the curves $B \sim Z^{4/3}B^*$ and $B \sim B^*Z^3$ and the expected domain of validity of the TF approximation for isolated atoms is shown in Fig. 8a. Note that TF theory is certainly bound to fail for $B > Z^3B^*$; such fields have been called "ultrastrong" [37, 3] or "superstrong" [4].

In bulk matter the Wigner-Seitz radius, r_c , enters as a new basic length. In terms of r_c , the volume per nucleus is $4\pi r_c^3/3$. In dense matter one has $r_c < Z^{-1/3}a_0$ and $r_c < (Za_0 l_B^2)^{1/5}$ by (3.33) and (3.34). The last condition may also be written $B < Z^{1/2}(a_0/r_c)^{5/2}B^*$. The strong field domain, where essentially only the lowest Landau band is populated is here characterized by $l_B < Z^{-1/3}r_c$, i.e., $Z^{2/3}(a_0/r_c)^2 B^* < B$. These conditions become a little more transparent if we introduce a dimensionless "compression parameter"

$$\alpha = Z^{-1/3}a_0/r_c; \quad (3.37)$$

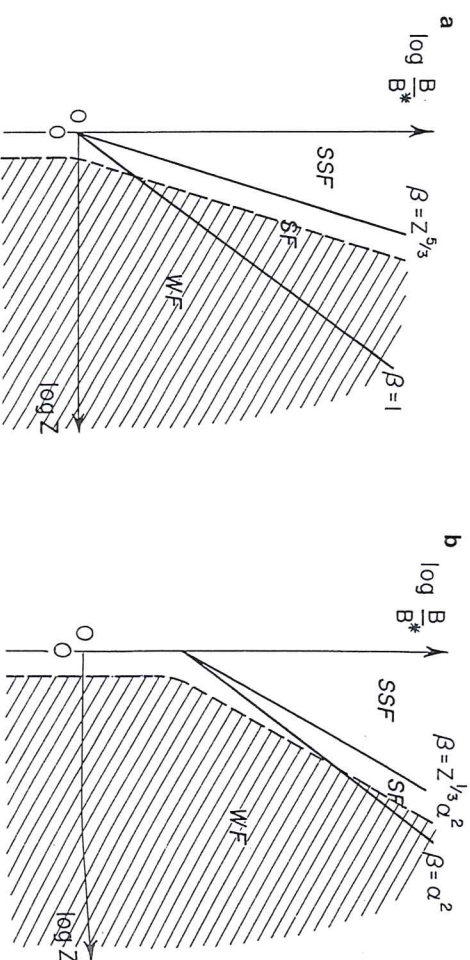


FIG. 8. (a) Z - B diagram for a single atom. WF: weak field, $\beta < 1$. SF: Strong field, $\beta > 1$. SSF: superstrong field, $\beta > Z^{5/3}$. (b) Z - B diagram for compressed matter, $\alpha > 1$, $\beta < \alpha^{5/2}$. WF: weak field, $\beta < \alpha^2$. SF: strong field, $\beta > \alpha^2$. SSF: superstrong field, $\beta > Z^{1/3}\alpha^2$. Shaded area: expected range of validity of the TF approximation.

the parameter range for "dense matter in a strong field" is now given by $\alpha > 1$ and

$$\alpha^2 Z^{4/3} B^* < B < \alpha^{5/2} Z^{4/3} B^*. \quad (3.38)$$

Within this range the condition for validity of the TF approximation is $\lambda_F \ll r_c$, or, equivalently,

$$B \ll B^* \alpha^2 Z^{5/3}. \quad (3.39)$$

In terms of the matter density $\rho := Am_p / (4\pi r_c^3 / 3)$ (A = atomic number, n_p = nucleon mass), one can write (3.38) as

$$(4\pi a_0 / 3m_p)^{2/3} B^* \frac{Z^{2/3}}{A} \rho^{2/3} < B < (4\pi a_0 / 3m_p)^{5/6} B^* \frac{Z^{1/2}}{A^{5/6}} \rho^{5/6} \quad (3.40)$$

and (3.39) as

$$B \ll (4\pi a_0 / 3m_p)^{2/3} B^* \frac{Z}{A^{2/3}} \rho^{2/3}. \quad (3.41)$$

(In [7], where (3.41) also occurs in a slightly different form, there is a misprint: The power of Z should there be $\frac{2}{3}$, not 2.)

It should be noted that outside the range of Eq. (3.38), i.e., for weak fields or isolated atoms, one can reasonably expect the previously discussed conditions to remain valid. For $B < \alpha^{5/2} Z^{4/3} B^*$ the condition is thus simply $Z^{-1/3} \ll 1$, and for $\alpha^2 Z^{4/3} B^* < B$ one should require $B \ll Z^3 B^*$. These conditions are illustrated in a Z - B diagram in Fig. 8b.

Using the parameter β instead of B one may summarize the preceding discussion as follows: TF theory of an atom is characterized by a single parameter β measuring the field strength, and bulk matter has essentially one additional parameter, the compression parameter α . Without restriction one can assume α to be no less than 1; bulk matter and single atoms can be discussed in a unified way if one defines $\alpha = 1$ for single atoms. In dense matter $\beta < \alpha^{5/2}$, and for $\alpha^2 < \beta$ we speak of *strong fields*. The quantum-mechanical ground state depends not only on α and β , but also in a nontrivial way on the nuclear charge Z . One expects TF theory to be a good approximation to quantum mechanics if

$$Z^{1/3} \gg \begin{cases} 1 & \text{for } \beta < \alpha^2 \\ \beta/\alpha^2 & \text{for } \alpha^2 < \beta < \alpha^{5/2} \\ \beta^{1/5} & \text{for } \alpha^{5/2} < \beta. \end{cases} \quad (3.42)$$

IV. HARTREE-FOCK ENERGY FOR THE HOMOGENEOUS ELECTRON GAS AND THOMAS-FERMI-DIRAC THEORY

In Thomas-Fermi-Dirac theory the energy density w includes not only the kinetic energy but also the exchange part of the Coulomb interaction for the

homogeneous electron gas. An account of TFD theory in the absence of a magnetic field may be found in, e.g., Gombás [17], Bethe and Jackiw [38], and Lieb [20]. The exchange energy in a strong magnetic field has been discussed by Danz and Glasser [39], Banerjee *et al.* [4], Rau *et al.* [16], Fushiki *et al.* [7], and used for TFD calculations of the properties of atoms and solids [2-7]. In these works the magnetic field was assumed to be so strong that only the lowest Landau band had to be considered.

In this section we discuss qualitative features of TFD theory of matter in a magnetic field allowing for occupancy of more than one Landau band. A measure of the importance of the exchange corrections is obtained by estimating the contribution the exchange energy makes to the total energy of matter. As in the case of TF theory, it is convenient to consider the limit of large Z for fixed $B/Z^{4/3}$. The size of the exchange hole around an electron has a characteristic size of order the inter-electron spacing, $\sim a_0/Z^{2/3}$, and therefore if the exchange energy may be treated as a perturbation its magnitude is $\sim Z^{2/3} e^2/a_0$ per electron or $\sim Z^{5/3} e^2/a_0$ per atom, which is $Z^{-2/3}$ times the leading contribution. One thus expects TFD theory to pass over into TF theory for $Z \rightarrow \infty$, in accordance with the limit theorems discussed in the last section. This is further substantiated by the considerations below.

The basic assumption of TF and TFD theory is that locally the energy density is given by that for a homogeneous electron gas, and the main part of this section is devoted to its computation in a Hartree-Fock approximation. In accordance with the basic assumption we can, in this computation, ignore inhomogeneous states such as charge density waves and Wigner crystals (see, e.g., [40-42]). A tendency to form inhomogeneous states is, however, latent in the homogeneous electron gas, for we show that it exhibits a first-order phase transition each time a new Landau band begins to be occupied. In TFD calculations these transitions lead to jumps in electron density profiles as discussed in Section II.

For the three-dimensional electron gas in the absence of a magnetic field translational invariance ensures that the self-consistent Hartree-Fock orbitals must be plane waves for all directions of the electron motion, which greatly simplifies the calculations. In the presence of a magnetic field only the motion along the field has plane wave character, while perpendicular to it the motion is more complicated, as described by the wave functions (3.2) in the absence of electron-electron interactions. The electron-electron interaction will generally alter the character of the orbitals perpendicular to the magnetic field. If, for example, the effect of the exchange interaction were simply to alter the effective mass, m^* , of electrons for motion perpendicular to the field, the wave functions would still be given by Eq. (3.2), but their energies for translational motion would be given by $(\alpha + \frac{1}{2}) \hbar \omega_B^*$, where $\omega_B^* = eB/(m^*c)$ is the renormalized cyclotron frequency. In general, the orbitals will be modified by the interaction, and their energies will be given by more complicated expressions. They will, however, still be degenerate with respect to the quantum number M . The calculation of the self-consistent orbitals is a difficult task which we shall not attempt here for two reasons. First, the exchange energy is generally a

minor contribution to the total energy. Second, we are particularly interested in exploring qualitative effects which occur when a new Landau band begins to be populated. These effects are associated with the motion along the field, and we do not expect their character to be influenced by modifications in the orbitals. We shall therefore perform a restricted Hartree-Fock calculation in which we assume that the single particle orbitals are given by Eq. (3.2). We note that the exchange potential depends explicitly on spin, since the populations of sub-bands of opposite spin differ, and this effect, as well as that associated with the translational motion discussed earlier, implies that the energies of orbitals (and their occupation numbers) do not depend on α and σ only in the combination $\alpha + \sigma$, as they did in the absence of the exchange interaction, cf. Eq. (3.4). This lifting of degeneracy, however, is a small effect that does not affect leading order calculations.

We turn now to the calculation of the energy in the Hartree-Fock approximation. The kinetic energy density is again given by Eq. (3.4). Here $\epsilon_{p\alpha\sigma}^0$ is the energy (3.1) of a free electron in a magnetic field, but the distribution function $n_{p\alpha\sigma}$ to be inserted here must be determined self-consistently, allowing for the effects of exchange. Next we consider the Coulomb interaction. Its long-range part will in the TFD calculation be taken care of by the term (2.5) in the energy functional, and for the homogeneous electron gas we assume that this part is compensated by a uniform neutralizing background of positive charge. Thus the interaction energy to be calculated in the Hartree-Fock approximation is the exchange energy, which is shown in Appendix A to be given by

$$W_{ex} = -\frac{1}{2} \sum_{pp'z\beta\sigma} V_{z\beta}(p-p') n_{p\alpha\sigma} n_{p'\beta\sigma\alpha} \quad (4.1)$$

with

$$V_{z\beta}(q) = 2\pi \int_0^\infty \rho d\rho \int_{-\infty}^{+\infty} dz e^{-\nu} L_\alpha(\nu) L_\beta(\nu) \frac{e^2}{(\rho^2 + z^2)^{1/2}} e^{-iqz/h}, \quad (4.2)$$

where $\nu = \rho^2/(2l_B^2)$ and L_α and L_β are Laguerre polynomials.

The matrix element, $V_{z\beta}$, may also be written as

$$V_{z\beta}(q) = 2\pi l_B^2 e^2 F_{z\beta}(\sqrt{2} ql_B/h), \quad (4.3)$$

where

$$F_{z\beta}(x) = 2 \int_0^\infty \xi d\xi \int_{-\infty}^\infty d\zeta \cos(2x\zeta) \frac{L_\alpha(\xi^2) L_\beta(\xi^2) e^{-\xi^2}}{(\xi^2 + \zeta^2)^{1/2}}. \quad (4.4)$$

The evaluation of $F_{z\beta}$ is described in Appendix B, and the results of numerical calculations of the functions F_{00} , F_{01} , and F_{11} are plotted in Fig. 9. For small x we have by Eq. (B.9),

$$F_{z\alpha}(x) = -\ln((\alpha+1)x^2) + O(1), \quad (4.5)$$

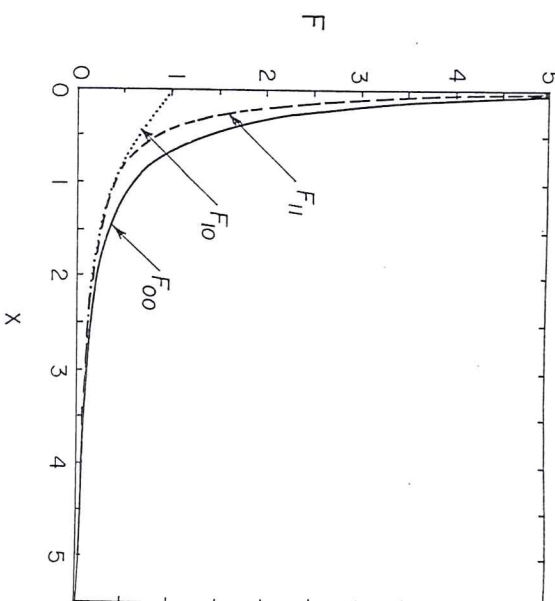


FIG. 9. The functions $F_{00}(x)$, $F_{01}(x) = F_{10}(x)$, $F_{11}(x)$.

whereas $F_{z\beta}$ stays bounded at zero if $\alpha \neq \beta$. For large x the functions $F_{z\beta}$ decrease as $1/x^2$.

The behaviour of $F_{z\beta}(x)$ for small x can be understood by noting that $V_{z\beta}(q) \cdot n^*$ is essentially the Coulomb energy of an electron at the origin interacting with a charge distribution of length $\sim h/q$ in the z direction, and whose distribution perpendicular to the field is given by $e^{-\nu} L_\alpha(\nu) L_\beta(\nu)$. For $\alpha = \beta$ the characteristic dimension of the distribution in the latter directions is of order of the cyclotron radius of an electron in level α , i.e., $(2\alpha+1)^{1/2} l_B$. Thus $V_{z\alpha} \cdot n^*$ is basically the potential at the center of a rod with length h/q , width $\sim (2\alpha+1)^{1/2} l_B$, and charge e/l_B per unit length. Hence,

$$V_{z\alpha}(q) \sim l_B^2 e^2 \ln[h/(2\alpha+1)^{1/2} l_B q] \quad (4.6)$$

for $q \ll h/(2\alpha+1)^{1/2} l_B$. If $\alpha \neq \beta$, the net charge associated with the distribution vanishes, because of the orthogonality of the Laguerre polynomials, and thus there is no logarithmic term.

To find the ground state in Hartree-Fock theory one must minimize the total energy density functional

$$W[n_{p\alpha\sigma}] = W_{kin}[n_{p\alpha\sigma}] + W_{ex}[n_{p\alpha\sigma}] \quad (4.7)$$

by varying $n_{p\alpha\sigma}$ subject to the constraint that the number density of electrons remain constant,

$$\sum_{p\alpha\sigma} n_{p\alpha\sigma} = n. \quad (4.8)$$

The minimization may be carried out in two stages: first, a minimization keeping fixed the total number of electrons in each Landau band, $n_{\alpha\sigma} = \sum_p n_{p\alpha\sigma}$; second, a minimization with respect to the populations of the bands, keeping fixed the total number of electrons $n = \sum_{\alpha\sigma} n_{\alpha\sigma}$.

Since the exchange interaction $-V_{\alpha\alpha}$ is a monotonically increasing function of $|q|$ it is simple to show that for a single Landau band the lowest energy state is achieved by filling all orbitals with momenta whose magnitudes are less than some value, p_F , the Fermi momentum for the band. For the case of many bands we shall assume that a similar result holds, with each band having its own Fermi momentum,

$$p_{F\alpha\sigma} = 2\pi^{-1/2} \hbar n_{\alpha\sigma} \quad (4.9)$$

(cf. Eq. (3.7)). This appears very plausible, and when exchange between different bands is ignored it can be verified by the same arguments as for a single band. Since exchange between bands plays no significant role in the considerations below, we feel justified in not presenting a formal proof for the general case.

If all distribution functions are of the form $n_{p\alpha\sigma} = \text{const} \cdot \theta(p_{F\alpha\sigma} - |p|)$, we can write

$$W_{\text{kin}} = \hbar\omega_B n_* \sum_{\alpha\sigma} \left[\left(\alpha + \sigma + \frac{1}{2} \right) x_{\alpha\sigma} + \frac{1}{3} x_{\alpha\sigma}^3 \right], \quad (4.10)$$

where $x_{\alpha\sigma} := n_{\alpha\sigma}/n_*$, and

$$W_{\text{ex}} = -\frac{\hbar\omega_B n_*}{2} \frac{l_B}{\sqrt{2}\pi} \left(\frac{l_B}{a_0} \right) \sum_{\alpha\beta\sigma} [F_{\alpha\beta}^{(2)}(x_{\alpha\sigma} + x_{\beta\sigma}) - F_{\alpha\beta}^{(2)}(|x_{\alpha\sigma} - x_{\beta\sigma}|)], \quad (4.11)$$

with

$$F_{\alpha\beta}^{(2)}(x) = \int_0^x \int_0^{x'} F_{\alpha\beta}(x'') dx' dx'' \quad (4.12)$$

For small $x_{\alpha\sigma}$ one has by (4.5)

$$F_{\alpha\alpha}^{(2)}(x_{\alpha\sigma}) = -2x_{\alpha\sigma}^2 \ln((\alpha+1)x_{\alpha\sigma}^2) + O(x_{\alpha\sigma}^2). \quad (4.13)$$

Moreover, for $\alpha \neq \beta$,

$$F_{\alpha\beta}^{(2)}(x_{\alpha\sigma} + x_{\beta\sigma}) - F_{\alpha\beta}^{(2)}(|x_{\alpha\sigma} - x_{\beta\sigma}|) = 2F_{\alpha\beta}^{(1)}(x_{\beta\sigma})x_{\alpha\sigma} + O(x_{\alpha\sigma}^2) \quad (4.14)$$

with

$$F_{\alpha\beta}^{(1)}(x) = dF_{\alpha\beta}^{(2)}(x)/dx = \int_0^x F_{\alpha\beta}(x') dx'. \quad (4.15)$$

Plots of $F_{\alpha\beta}^{(1)}$ and $F_{\alpha\beta}^{(2)}$ for the lowest values of α and β are shown in Figs. 10 and 11.

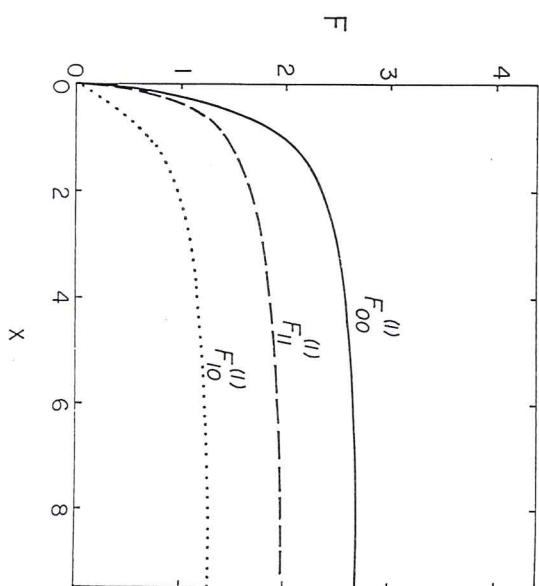


FIG. 10. The functions $F_{00}^{(1)}(x)$, $F_{01}^{(1)}(x) = F_{10}^{(1)}(x)$, $F_{11}^{(1)}(x)$.

The chemical potential of band $\alpha\sigma$ is

$$\begin{aligned} \mu_{\alpha\sigma} &= \frac{\partial W[n_{\alpha\sigma}]}{\partial n_{\alpha\sigma}} \\ &= \hbar\omega_B \left[\left(\alpha + \sigma + \frac{1}{2} \right) + x_{\alpha\sigma}^2 - \frac{1}{2\sqrt{2}\pi} \left(\frac{l_B}{a_0} \right) \right. \\ &\quad \left. \times \sum_{\beta} [F_{\alpha\beta}^{(1)}(x_{\alpha\sigma} + x_{\beta\sigma}) - \varepsilon(x_{\alpha\sigma} - x_{\beta\sigma}) F_{\alpha\beta}^{(1)}(|x_{\alpha\sigma} - x_{\beta\sigma}|)] \right], \end{aligned} \quad (4.16)$$

where $\varepsilon(x)$ is the step function with value +1 for $x > 0$ and -1 for $x < 0$. For small $x_{\alpha\sigma}$

$$F_{\alpha\alpha}^{(1)}(2x_{\alpha\sigma}) = -2x_{\alpha\sigma} \ln((\alpha+1)x_{\alpha\sigma}^2) + O(x_{\alpha\sigma}) \quad (4.17)$$

by (4.5), and

$$\begin{aligned} F_{\alpha\beta}^{(1)}(x_{\alpha\sigma} + x_{\beta\sigma}) - \varepsilon(x_{\alpha\sigma} - x_{\beta\sigma}) F_{\alpha\beta}^{(1)}(|x_{\alpha\sigma} - x_{\beta\sigma}|) \\ = 2F_{\alpha\beta}(x_{\beta\sigma}) + O(x_{\alpha\sigma}^2) \end{aligned} \quad (4.18)$$

if $\alpha \neq \beta$.

Returning now to the second stage of the minimization, a necessary condition for the ground state to satisfy is that the chemical potentials of all populated bands are equal,

$$\mu_{\alpha\sigma} = \mu, \quad (4.19)$$

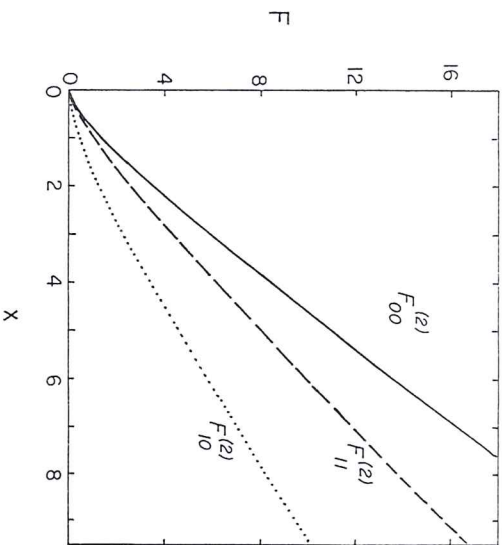


Fig. 11. The functions $F_{00}^{(2)}(x)$, $F_{01}^{(2)}(x) = F_{10}^{(2)}(x)$, $F_{11}^{(2)}(x)$.

for all $\alpha\sigma$ such that $n_{\alpha\sigma} > 0$, where μ is a common chemical potential. Moreover, a band $\alpha'\sigma'$ is empty only if its chemical potential, evaluated at $n_{\alpha'\sigma'} = 0$, is larger than μ .

A somewhat unexpected result is that there can be multiple solutions to these equations, corresponding to different local minima of the energy, for fixed total density. The basic reason for this is that the chemical potential of each band has a negative slope for low densities in the band, due to the exchange interaction. To explore these solutions in more detail we shall restrict ourselves to the case of fields

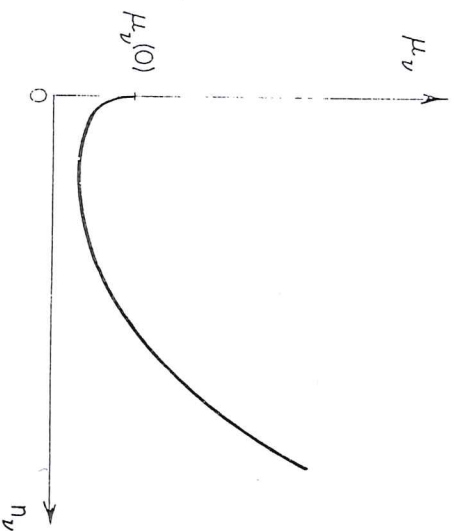


Fig. 12. Sketch of the chemical potential, $\mu_v = \mu_v(n_v)$, in a band with a low population.

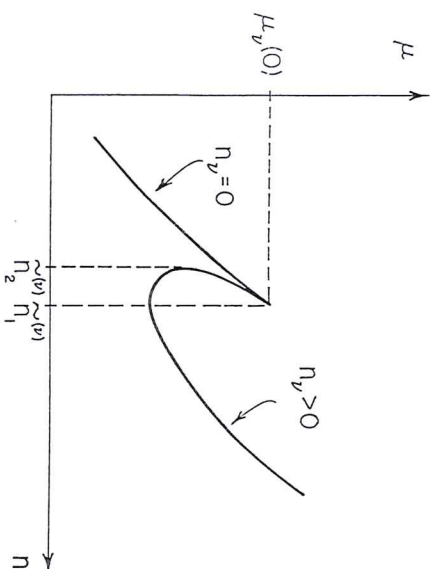


Fig. 13. Schematic picture of the chemical potential, μ , versus total density, n , for the model discussed in the text.

sufficiently strong that l_B/a_0 may be regarded as a small parameter and consider only the Landau levels $\alpha\sigma$ with $l_B/a_0 \ll (\alpha + 1)^{-1/2}$. (Note that the restriction on B does not exclude that the field is "weak" in the sense of Section III if Z is sufficiently high and/or matter compressed, because $l_B/a_0 = (B/B^*)^{-1/2} = \beta^{-1/2} Z^{-2/3}$.)

By Eqs. (4.16)-(4.18) one can in leading approximation assume that the chemical potential of a band $\alpha\sigma$ with a low population is a function of $n_{\alpha\sigma}$ alone. Moreover, to the same accuracy one can as in the free case index the bands by $v = \alpha + \sigma + \frac{1}{2}$,

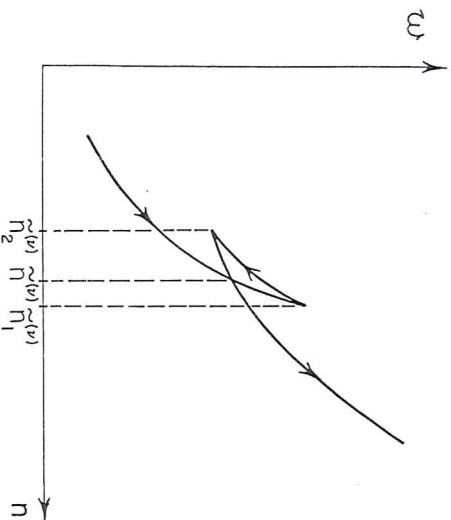


Fig. 14. Schematic picture of the energy function, w , versus total density, n , obtained by integrating $\mu(n) = w'$ shown in Fig. 13. The lowest Hartree-Fock energy density, $w = w(n)$, is obtained by cutting off the "swallowtail."

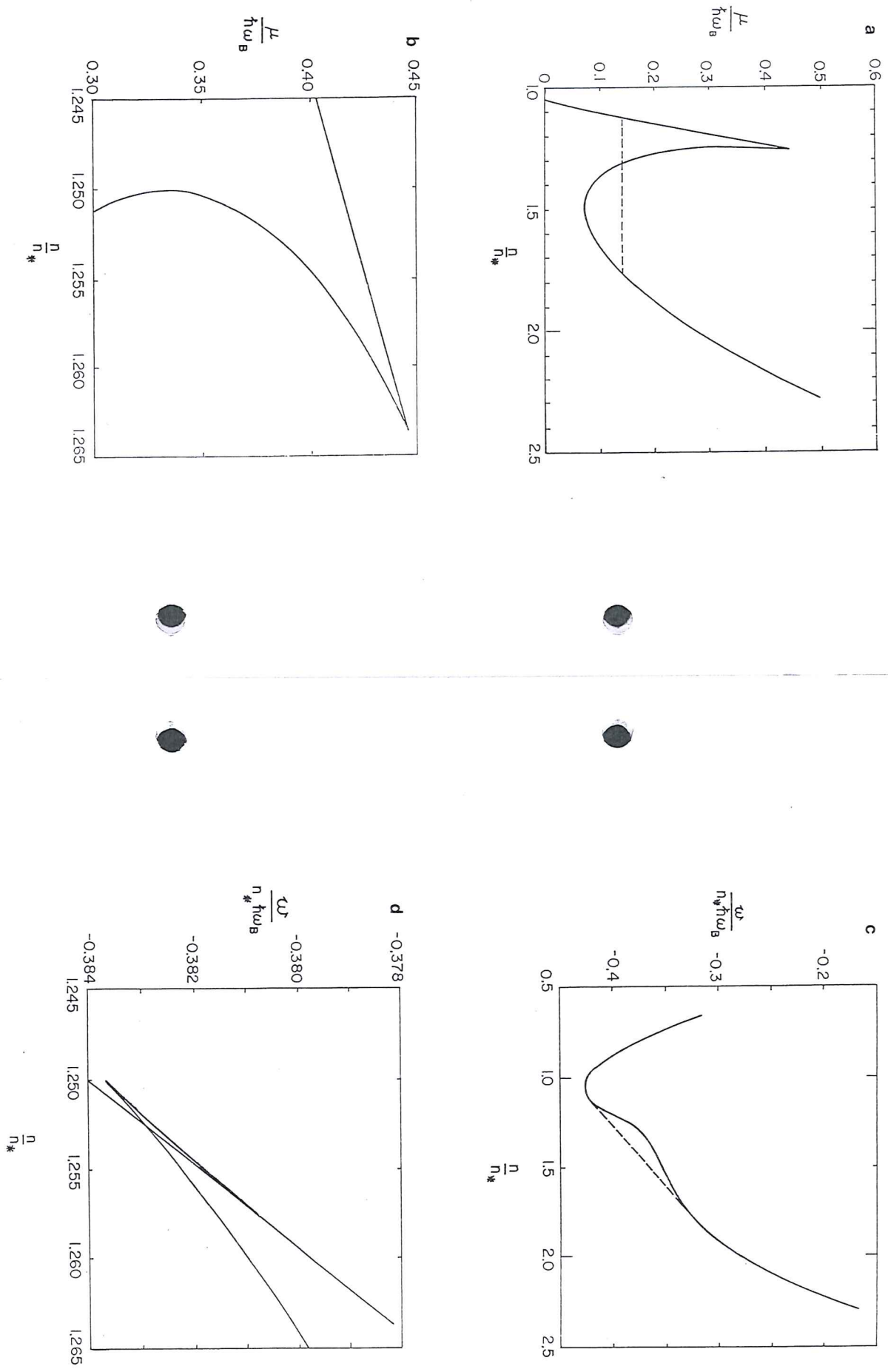


Fig. 15. Numerical solutions to the Hartree-Fock equations for the homogeneous electron gas for $v = 1$ and $B = 10^8$ gauss. (a) The chemical potential, μ . (b) Blowup of the curve in (a). (c) The energy density, ω . (d) Blowup of the curve in (c).

FIGURE 15—Continued

keeping in mind that the all energy levels with $\nu \geq 1$ count double. The chemical potential of band ν can then approximately be written

$$\mu_\nu(x_\nu) = \mu_\nu(0) + \hbar\omega_B \left[c_\nu x_\nu^2 + \frac{(2c_\nu)^{1/2}}{\pi} \left(\frac{l_B}{a_0} \right) x_\nu \ln((\nu+1)^{1/2} x_\nu) \right], \quad (4.20)$$

where $x_\nu = n_\nu/n_*$, and $c_0 = 1$, $c_\nu = 1/4$ for $\nu \geq 1$. A sketch of μ_ν is shown in Fig. 12. The minimum of (4.20) is for $l_B/a_0 \ll (\nu+1)^{-1/2}$ obtained at

$$x_\nu = O(1)(l_B/a_0) \ln[a_0/((\nu+1)^{1/2} l_B)], \quad (4.21)$$

so the lowest energy of the band is

$$(\mu_\nu)_{\min} = \mu_\nu(0) - O(1)\hbar\omega_B(l_B/a_0)^2 \ln^2[a_0/((\nu+1)^{1/2} l_B)]. \quad (4.22)$$

Now suppose $\nu \geq 1$ and let us imagine that we start with a chemical potential slightly below the bottom of band ν and gradually add electrons, at first to the bands with index lower than ν . Then $\mu(n)$ will increase until n takes on the value, $\tilde{n}_1^{(\nu)}$, for which $\mu(\tilde{n}_1^{(\nu)}) = \mu_\nu(0)$. Since the exchange contributions to the chemical potential are negative, these densities are slightly higher than the threshold densities $n^{(\nu)}$ for the free case considered in Section III. If we now put a few electrons into band ν , μ_ν will at first decrease and the equilibrium condition $\mu = \mu_\nu$ can be satisfied only by removing electrons from the lower bands. Since for small n_ν the negative slope of μ_ν as a function of density is larger than the positive slope of μ for the lower bands at the equilibrium value $\mu = \mu_\nu$, more electrons have to be removed from the lower bands than are put into the higher one. Thus the total number density decreases and so does the chemical potential. This is demonstrated in Fig. 13 which shows μ as a (multivalued) function of the total density n . The decrease of n stops at the value $\tilde{n}_2^{(\nu)}$ where the negative slope of the chemical potential of band ν is matched by the positive slope of the potential for the lower bands, but μ keeps decreasing for a while until finally it starts to bend upwards again when the bottom of band ν is reached.

Since $\mu = d\mathcal{w}/dn$ we can also use Fig. 13 to draw a schematic picture of \mathcal{w} . The result is shown in Fig. 14 and the results of a numerical calculation for $\nu = 1$, in Fig. 15. The "swallowtail" of the \mathcal{w} curve corresponds to the backward bending of the μ curve. For the corresponding total electron densities the energy density has at least two local minima as a function of the populations of the individual bands. The lowest Hartree-Fock energy density is obtained by cutting off all swallowtails.

From these considerations it is also clear that $\mathcal{w}(n)$, with the tails removed, is a non-convex function of n in the neighborhood of each of the threshold densities. The chemical potential $\mu(n) = d\mathcal{w}(n)/dn$, drops discontinuously at each of the critical densities $\tilde{n}^{(\nu)}$, where the lowest branches of \mathcal{w} cross, and the electron population in the higher band increases discontinuously from zero to a finite value. The densities $\tilde{n}^{(\nu)}$ are determined by an equal area construction in the μn plane, cf. Fig. 16a.

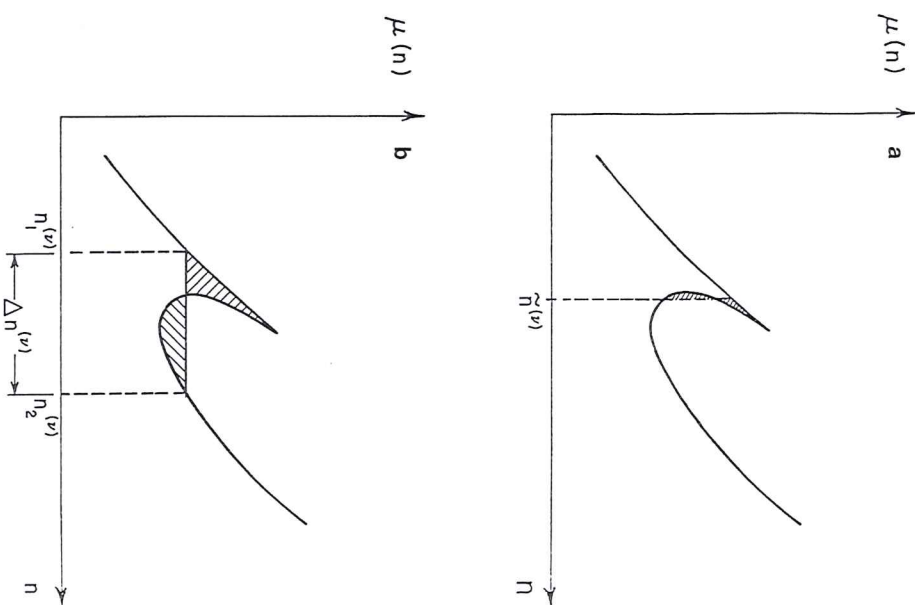


FIG. 16. (a) Equal area construction to determine $\tilde{n}^{(\nu)}$. In a $\mu(n)$ plot, the density $\tilde{n}^{(\nu)}$ at which the occupation of the second level increases discontinuously is determined by the equal area construction as shown in the figure. Note that there is a discontinuous jump in μ at the critical density $\tilde{n}^{(\nu)}$. (b) Equal area construction to determine the density jump $d\tilde{n}^{(\nu)}$.

As discussed in Section II the relevant energy density for TFD calculations is actually the convex hull of \mathcal{w} , obtained by a double tangent construction from the graph of \mathcal{w} as shown in Fig. 17, or equivalently, by an equal area construction as in Fig. 16b. The flat portions of the corresponding chemical potential can be interpreted as first-order phase transitions of the homogeneous electron gas. In TFD calculations these transitions lead to jumps in the electron densities.

We now estimate the size of the singular features in the graphs of μ and \mathcal{w} . Consider first the width of the swallowtail, $\Delta\tilde{n}^{(\nu)} = \tilde{n}_1^{(\nu)} - \tilde{n}_2^{(\nu)}$. The slope of $\mu/\hbar\omega_B$ as a function of the density in bands lower than ν is of the order $O(1)(\nu+1)^{-1/2}$ in the

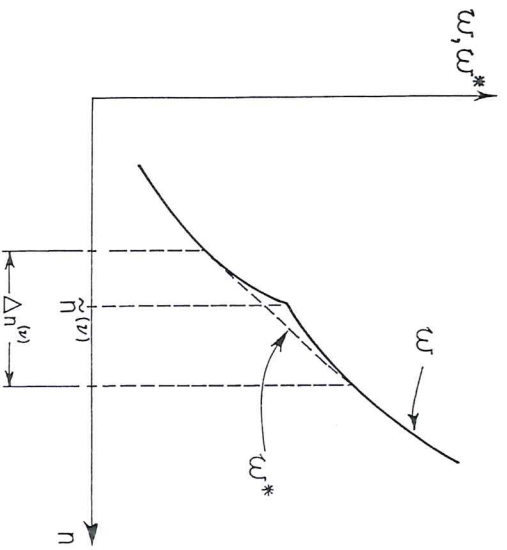


Fig. 17. The convex hull, ω^* , of the energy function, ω ; for the model discussed in the text. ω^* is obtained by means of a double tangent construction. The density jump, $\Delta n^{(v)}$, is indicated in the figure.

neighbourhood of $\tilde{n}_1^{(v)} \approx n^{(v)}$, cf. Eq. (3.17). If $l_B/a_0 \ll (\nu+1)^{-1/2}$, then this slope matches the slope of μ_v for

$$x_v = O(1)(\nu+1)^{-1/2} \exp[-O(1)a_0/((\nu+1)^{1/2}l_B)], \quad (4.23)$$

with a corresponding value of the chemical potential

$$\mu_v = \mu_v(0) - h\omega_B O(1)(\nu+1)^{-1} \exp[-O(1)a_0/((\nu+1)^{1/2}l_B)]. \quad (4.24)$$

Hence,

$$\Delta \tilde{n}^{(v)}/n_* = O(1)(\nu+1)^{-1/2} \exp[-O(1)a_0/((\nu+1)^{1/2}l_B)]. \quad (4.25)$$

The density jumps $\Delta n^{(v)} = n_2^{(v)} - n_1^{(v)}$ associated with the phase transitions (see Figs. 16b and 17) are estimated by equating chemical potentials and pressures at $n_1^{(v)}$ and $n_2^{(v)}$. By (2.11) the pressure is $P = \mu n - w$. Since the chemical potentials are equal and the contribution of the higher band to the energy is additive, the equilibrium condition for the pressure means simply that the partial pressure of the higher band must vanish:

$$\mu_v(x_v) x_v - \int_0^{x_v} \mu_v(x) dx = 0. \quad (4.26)$$

Moreover, the population of the lower bands does not change, while that of band ν jumps by $\Delta n^{(v)} = n_* x_v$. With (4.20) one finds

$$\Delta n^{(v)}/n_* = O(1)(l_B/a_0) \ln[a_0/((\nu+1)^{1/2}l_B)]. \quad (4.27)$$

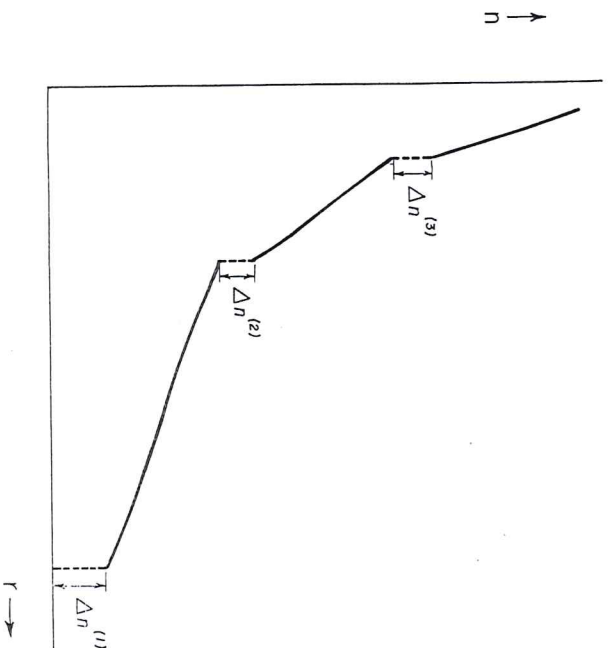


Fig. 18. Schematic density profile of an atom in a magnetic field, obtained in a TFD calculation.

Since $l_B/a_0 = \beta^{-1/2} Z^{-2/3}$, this can also be written as

$$\Delta n^{(v)}/n_* = O(1) \beta^{-1/2} Z^{-2/3} \ln[\beta Z/((\nu+1)^{1/2})]. \quad (4.28)$$

In Fig. 18 we show schematically an atomic profile in TFD theory with $\beta \approx 1$. The smoothing effect of a von Weizsäcker term in the energy functional on the discontinuities will be discussed in the next section.

V. GRADIENT CORRECTIONS

Thomas-Fermi theory rests on the assumption that the electronic density varies slowly on length scales characteristic of the electron gas, such as a typical inter-electronic distance. This condition is not always fulfilled, and, to overcome this deficiency of the theory, von Weizsäcker [43] added to the TF energy functional for zero magnetic field a correction term of the form

$$\mathcal{E}_{gr}[n] = \frac{\hbar^2 \xi}{8m} \int d^3r \frac{(\nabla n(\mathbf{r}))^2}{n(\mathbf{r})}, \quad (5.1)$$

where ξ is a number of order unity. For density fluctuations of small amplitude

whose spatial scale is small compared with the Fermi wavelength, von Weizsäcker argued that $\xi = 1$. For the case of finite magnetic field, this result still holds, provided the scale of density variations is small compared with the Fermi wavelengths and the magnetic length, l_B , as we now show. Following, e.g., Jones and Gunnarsson ([28, Section II.B2]) the change in the energy density of a non-interacting electron gas when there is a small density variation is given by

$$\delta E = \frac{1}{2} \sum_q \frac{|\delta n_q|^2}{\chi(q)}, \quad (5.2)$$

where δn_q is the Fourier transform of the density fluctuation and $\chi(q)$ is the static density-density response function of the free electron gas given by

$$\chi(q) = \sum_k \frac{2 |(n_q)_{k0}|^2}{\omega_{k0}}. \quad (5.3)$$

Here $\omega_{k0} = \epsilon_k - \epsilon_0$ is the energy of the excited state, k , relative to that of the ground state, and n_q is the Fourier transform of the electron density operator.

When the wavelength $2\pi/q$ is small compared with Fermi wavelengths and the magnetic length, the electron wavefunctions behave as plane waves on length scales $\sim 2\pi/q$. Consequently the leading contribution to the excitation energies for $q \rightarrow \infty$ is the recoil energy, $\hbar^2 q^2/2m$. Thus we may write

$$\chi(q) = \sum_k \frac{2\omega_{k0} |(n_q)_{k0}|^2}{\omega_{k0}^2} \rightarrow \sum_k \frac{2\omega_{k0} |(n_q)_{k0}|^2}{(\hbar^2 q^2/2m)^2}. \quad (5.4)$$

From the f -sum rule (see, e.g., [44]) the numerator is $nh^2 q^2/m$, and thus

$$\chi^{-1}(q) \rightarrow \frac{\hbar^2 q^2}{4\pi m}, \quad (5.5)$$

and the expression (5.2) then reduces to the form of Eq. (5.1), with $\xi = 1$.

The arguments given above demonstrate that, for short wavelength density fluctuations, the von Weizsäcker term does not depend on the magnetic field. This conclusion has also been reached recently by Abraham and Shapiro [25] by a direct generalization of von Weizsäcker's original argument. For zero field another expression for the von Weizsäcker term has been derived by considering long-wavelength fluctuations, as discussed, e.g., in [28], and one finds that the coefficient ξ is $\frac{1}{2}$. If one carries out the analogous calculations for electrons in a magnetic field, one finds that the von Weizsäcker term is no longer isotropic, but may be written in the form

$$\frac{\hbar^2}{2m} \int dt [f_{\parallel}(n, B)(\nabla_{\parallel} n)^2 + f_{\perp}(n, B)(\nabla_{\perp} n)^2], \quad (5.6)$$

where ∇_{\parallel} and ∇_{\perp} are the components of the gradient in directions of the field and

perpendicular to it, respectively. The anisotropic form reflects that there are two sets of microscopic lengths in the problem, the Fermi wavelengths which are important for density variations along the direction of the field, and the magnetic length, which is important for variations perpendicular to the field. The functions f_{\parallel} and f_{\perp} have a rather complicated dependence on n and B , and they may be determined from results for the density-density response function χ in a magnetic field, which has been explored in some detail by Yakovlev and Shalybkov [45]. One interesting fact is that f_{\parallel} can be negative.

Let us now estimate how the von Weizsäcker term for small wavelength fluctuations (5.1) will affect electron density profiles. When it is included in TF calculations it leads to the integro-differential equation

$$\frac{\hbar^2 \xi}{8m} \frac{(\nabla n)^2}{n^2} - \frac{\hbar^2 \xi}{4m} \frac{\nabla^2 n}{n} + \mu(n) = \mu_{\text{cl}} + e\Phi, \quad (5.7)$$

which should be compared with Eqs. (2.9) and (2.16). The von Weizsäcker term has the effect of smoothing out density profiles. In particular near a nucleus the density tends to a constant, rather than diverging as it does in TF theory. The von Weizsäcker term will lead to an energy per particle of order $\hbar^2/(2ml^2)$, where l is the characteristic length in spatial variations of the density. Near the nucleus this term will become comparable to the electrostatic energy, which tends to the bare Coulomb energy Ze/lr if $r \sim l \sim a_0/Z$. The volume within radius l contains ~ 1 electron, and the contribution to the total energy from the von Weizsäcker term is of order $\hbar^2/(2ml^2) \sim Z^2 e^2/a_0$, compared with the TF energy which varies as $Z^{7/3}$.

That the von Weizsäcker term gives corrections of order Z^2 has been shown rigorously for the case of zero field by Lieb [20], and the qualitative behavior of this correction is the same as Scott [46] conjectured for the leading correction to TF theory in a full quantum-mechanical treatment (see also Lieb [20]). The Scott conjecture has recently been proven for atoms in zero magnetic field [47]. The corresponding result with a magnetic field would be

$$E^{\text{QM}}(Z, B) = Z^{7/3} E^{\text{TF}}(\beta) + Z^{-1/3} E_1(\beta) + O(Z^{-2/3}) \quad (5.8)$$

but this has still to be rigorously demonstrated.

The features of density profiles where new Landau bands begin to be occupied are also smoothed out by the von Weizsäcker term. Consider the square-root singularity in TF theory shown schematically in Fig. 19. One may estimate the characteristic length over which the singularity in the TF theory is smoothed by arguing that in TFW theory the von Weizsäcker energy must be comparable to the difference in electrostatic potential across the region. Since the electric field is of order $Ze/(a_0/Z^{1/3})^2 \sim Z^{5/3}e/a_0^2$, this condition gives

$$\hbar^2/(2ml^2) \sim Z^{5/3}e^2/l/a_0^2 \quad (5.9)$$

or

$$l \sim a_0/Z^{5/9}. \quad (5.10)$$

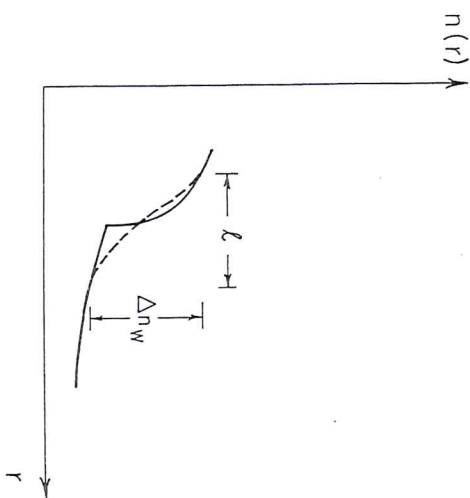


FIG. 19. The figure indicates the smoothing out of the infinities in the slopes of TF density profiles when a von Weizsäcker term is introduced in the calculation of an atomic profile.

In TF theory the density behaves as (see Eq. (3.26b))

$$(n - n_*^{(v)}) \sim \beta \frac{Z^2}{a_3^2} [Z^{1/3}(r^{(v)} - r)]^{1/2}, \quad (5.11)$$

and therefore the interval Δn_W , where the density is appreciably modified by the von Weizsäcker term, is given by

$$\frac{\Delta n_W}{n_*} \sim \beta^{-1/2} Z^{-1/9}. \quad (5.12)$$

Thus the fraction of the profile over which the smoothing is important tends to zero, albeit rather slowly, for $Z \rightarrow \infty$. We also note that the density range over which one expects smoothing exceeds the magnitude of density discontinuities in TFD theory, since $\Delta n_W \sim Z^{5/9} \Delta n^{(v)}$, cf. Eq. (4.28). The exchange energy will therefore have only minor effects on the density profiles calculated in TFW theory. In the limit $Z \rightarrow \infty$ with β fixed, the gradient correction vanishes and divergences in the density gradients reappear at the densities $n_*^{(v)}$.

VI. CONCLUDING REMARKS

In this paper we have studied a number of general features of TF-type theories of matter in a magnetic field, placing particular emphasis on the case when more than one Landau band is occupied. For ordinary TF theory, in which the effects of

exchange are neglected, we have shown that the ground state energy and electron density have simple transformation properties if the nuclear charges and the magnetic field are scaled simultaneously. Simple estimates of corrections to TF theory suggest that these should be small in the limit as the nuclear charges tend to infinity. In fact, the quantum mechanical limit theorems for zero magnetic field [18-21] have recently been generalized to the case where a magnetic field is present [22], establishing rigorously that TF theory with a magnetic field is a scaling limit of quantum mechanics.

In high magnetic fields, electron density profiles calculated in the TF approximation exhibit a shell structure distinct from that which exists in the full quantum mechanical treatment for zero field. Our estimates of the range of validity of TF theory and the rigorous limit theorems of [22] suggest that, for heavy atoms and field strengths in a certain range determined by the nuclear charge, this shell structure is real, and not just an artefact of the TF approximation. Detailed numerical calculations of density profiles and thermodynamic properties in TF theory are being carried out by Ö. E. Rögnvaldsson and will be reported in a separate publication. As a consequence of the singular features in density profiles in TF theory, one might expect singularities in the equation of state of bulk matter. However, these turn out to be weak, and the density is a smooth function of the pressure, with an oscillating component, which is the high field manifestation of the de Haas-van Alphen and related effects that are more familiar in the case when rather many Landau bands are occupied. To what extent TF calculations are a reliable guide to the magnitude of these effects in matter with large nuclear charges remains an open question.

A further remark on TF theory is that the scaling relations may be extended to finite temperatures. The temperature must be scaled so that the ratio of the thermal de Broglie wavelength, $\sim T^{-1/2}$, to the magnetic length, $\sim B^{-1/2}$, remains constant. Thus T should be scaled as B , that is, as $Z^{4/3}$. This result generalizes, to the case of many Landau bands, one of the scaling relations derived by Abrahams and Shapiro [25] for the case when a single Landau band is occupied.

As a preliminary to our study of TFD theory we investigated the exchange energy of the uniform gas. We obtained expressions for the exchange energy which are a generalization of earlier results for the case when only the lowest Landau band is occupied. It was also shown that the uniform electron gas, with a background of positive charge, exhibits first-order phase transitions as a function of electron density. These are Peierls-type instabilities associated with motion parallel to the magnetic field, and they are therefore distinct from density modulations in the direction perpendicular to the field found in two-dimensional systems in a magnetic field.

We have also drawn attention to the fact that there is no molecular binding in TF theories of matter in a magnetic field. This result follows quite generally from the earlier studies of Lieb, Simon, and Benguria, and it implies that TF-type theories are too crude to yield any information about a zero pressure state of dense matter in high magnetic fields.

Some shortcomings of TF theory may be remedied in a somewhat ad hoc manner by inclusion of a von Weizsäcker term. As in the case of zero field, a rigorous justification for such a theory does not exist, and there are various ways of choosing coefficients of the gradient term. One complication in the case of a finite field is that the von Weizsäcker term is generally anisotropic, and for gradients of the density parallel to the magnetic field, it can be negative. The utility of a theory of this type is somewhat limited at present, since there are few quantum-mechanical calculations of matter in a high field that can give guidance as to the choice of the von Weizsäcker term.

APPENDIX A: CALCULATION OF THE EXCHANGE ENERGY

In this appendix we show that the exchange energy is given by (4.1) and (4.2). In the uniform state, the electron distribution function is independent of M . Thus the exchange energy may be written as

$$W_{\text{ex}} = -\frac{1}{2} \sum_{p'p''\alpha'\alpha''M'M''} \langle p\alpha M, p'\alpha'M' | V | p'\alpha'\sigma'M', p\alpha M \rangle n_{p\alpha\sigma} n_{p'\alpha'\sigma}, \quad (\text{A.1})$$

where V is the Coulomb interaction potential. This is precisely of the form (4.1), with

$$\begin{aligned} V_{\alpha\beta}(p-p')\delta_{\sigma\sigma'} &= \sum_{MM'} \langle p\alpha M, p'\beta\sigma'M' | V | p'\beta\sigma'M', p\alpha M \rangle \\ &= \sum_{MM'} \int d^3\mathbf{r} d^3\mathbf{r}' \psi_{p\alpha M}^*(\mathbf{r}') \psi_{p'\beta\sigma'M'}^*(\mathbf{r}) \\ &\quad \times \frac{e^2}{|\mathbf{r}-\mathbf{r}'|} \psi_{p'\beta\sigma'M'}(\mathbf{r}') \psi_{p\alpha M}(\mathbf{r}). \end{aligned} \quad (\text{A.2})$$

The quantity

$$\sum_M \psi_{p\alpha M}^*(\mathbf{r}') \psi_{p\alpha M}(\mathbf{r}) = J_{p\alpha}(\mathbf{r}, \mathbf{r}') \quad (\text{A.3})$$

may be evaluated by inserting the wavefunctions (3.2) and using the identities

$$\begin{aligned} L_n^j(x) L_n^j(y) &= \frac{(n+j)!}{n!} \sum_{l=0}^n \frac{L_{n-l}^{j+2l}(x+y) (xy)^l}{(l+j)! l!}, \\ L_n^j(x+y) &= e^x \sum_{k=0}^{\infty} \frac{(-1)^k}{k!} y^k L_{n-k}^{j+k}(x) \\ &= \sum_{k=0}^n \frac{(-1)^k}{k!} y^k L_{n-k}^k(x). \end{aligned} \quad (\text{A.4})$$

After a simple computation one obtains (cf. also Ando *et al.* [48, Eq. (6.14)])

$$\begin{aligned} J_{p\alpha}(\mathbf{r}, \mathbf{r}') &= \frac{1}{2\pi l_B^2 L} e^{i\mathbf{l}(\mathbf{r}_\perp \times \mathbf{r}'_\perp) \cdot 2l/2l_B^2} e^{i\mathbf{l}p(z-z')/h} \\ &\quad \times L_\alpha((\mathbf{r}_\perp - \mathbf{r}'_\perp)^2/2l_B^2) \exp(-(\mathbf{r}_\perp - \mathbf{r}'_\perp)^2/4l_B^2), \end{aligned} \quad (\text{A.5})$$

where \hat{z} is the unit vector in the direction of the field, z the component of \mathbf{r} in this direction, and \mathbf{r}_\perp is the component, perpendicular to the field. The L_α 's are Laguerre polynomials, normalized as in [35, p. 775], i.e., $L_\alpha(0) = 1$.

The form of $J_{p\alpha}$ can also be deduced by general gauge invariance arguments, which are discussed for the case of the single-particle propagator by Horing [49] and Schwinger [50]. In gauges other than the symmetric one the dependence on $(\mathbf{r}_\perp - \mathbf{r}'_\perp)$ and $(z - z')$ is the same as in (A.5), but the phase factor will be different. Formulas (4.1)-(4.2) for the exchange energy follow immediately from Eqs. (A.2) and (A.5).

APPENDIX B: THE FUNCTIONS $F_{\alpha\beta}$, $F_{\alpha\beta}^{(1)}$ AND $F_{\alpha\beta}^{(2)}$

The function $F_{\alpha\beta}$ that determines the exchange energy between Landau levels α and β is given by (4.4). The integral over ξ can be performed using [51, p. 1151],

$$\int_{-\infty}^{\infty} \frac{\cos(2x\xi)}{(\xi^2 + z^2)^{1/2}} d\xi = 2K_0(2xz), \quad (\text{B.1})$$

with the Bessel function K_0 behaving as

$$K_0(z) = -\ln \frac{z}{2} + O(1) \quad (\text{B.2})$$

for small z . To carry out the integration over ξ^2 it is convenient to use the generating function for the Laguerre polynomials, cf. [35, p. 784]:

$$U(y, s) = \sum_{\alpha=0}^{\infty} L_\alpha(y) s^\alpha = \frac{\exp(-ys/(1-s))}{1-s}, \quad 0 \leq s < 1. \quad (\text{B.3})$$

One thus considers

$$\begin{aligned} I(x; s, t) &= 2 \int_0^\infty dy e^{-y} U(y, s) U(y, t) K_0(2x\sqrt{y}) \\ &= \frac{2}{(1-s)(1-t)} \int_0^\infty dy e^{-y t/(s,t)} K_0(2x\sqrt{y}), \end{aligned} \quad (\text{B.4})$$

with

$$a(s, t) = 1 + \frac{s}{1-s} + \frac{t}{1-t} = \frac{1-st}{(1-s)(1-t)}. \tag{B.5}$$

Using [51, pp. 709, 1060], one obtains

$$I(x; s, t) = \frac{1}{1-st} \exp(x^2/a(s, t)) E_1(x^2/a(s, t)) \tag{B.6}$$

with

$$E_1(z) = \int_z^\infty \frac{e^{-u}}{u} du = -\gamma - \ln z - \sum_{n=1}^\infty \frac{(-1)^n z^n}{n n!} \tag{B.7}$$

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

After series expansion in s and t one obtains $F_{\alpha\beta}(x)$ as the coefficient of $s^\alpha t^\beta$ in (B.6). Since

$$\begin{aligned} (1-st)^{-1} \ln(1-st) &= - \sum_{\alpha=1}^\infty \left(\sum_{k=1}^\alpha \frac{1}{k} \right) (st)^\alpha \\ &= - \sum_{\alpha=1}^\infty (\ln \alpha + \gamma + O(1/\alpha)) (st)^\alpha, \end{aligned} \tag{B.8}$$

we have

$$F_{\alpha\beta}(x) = -\ln((\alpha+1)x^2) + O(1) \tag{B.9}$$

for $(\alpha+1)x^2$ small, $\alpha \geq 0$, where the $O(1)$ -term is uniformly bounded in x and α . On the other hand, because $(1-st)^{-1} = \sum_x (st)^x$, it is clear that if $\alpha \neq \beta$ then $F_{\alpha\beta}$ has no logarithmic term and stays, therefore, bounded at zero.

By writing (B.6) in the form

$$\begin{aligned} I(x; s, t) &= \frac{1}{1-st} \int_0^x \frac{e^{-u}}{(x^2/a(s, t)) + u} du \\ &= \sum_{\alpha, \beta=0}^\infty \frac{s^\alpha t^\beta}{x^2} \int_0^x \frac{e^{-u}}{1 + (a(s, t)u/x^2)} du, \end{aligned} \tag{B.10}$$

one sees that

$$F_{\alpha\beta}(x) = \frac{1}{x^2} + O\left(\frac{1}{x^4}\right) \tag{B.11}$$

for large x . In particular, the functions

$$F_{\alpha\beta}^{(1)}(x) = \int_0^x F_{\alpha\beta}(x') dx' \tag{B.12}$$

that enter in the formula (4.16) for the chemical potentials have a finite limit for $x \rightarrow \infty$, and the functions

$$F_{\alpha\beta}^{(2)}(x) = \int_0^x F_{\alpha\beta}^{(1)}(x') dx' \tag{B.13}$$

grow linearly with x for large x .

To evaluate $F_{\alpha\beta}(x)$ more completely one may expand the integrand in (B.10), obtaining

$$F_{\alpha\beta}(x) = \sum_{\lambda=|\alpha-\beta|}^{\alpha+\beta} A_{\alpha\beta\lambda} x^{2\lambda} \int_0^{\infty} \frac{e^{-u}}{(x^2+u)^{\lambda+1}} du, \tag{B.14}$$

where

$$A_{\alpha\beta\lambda} = (-1)^{\alpha+\beta+\lambda} \sum_{k=0}^{\min(\alpha, \beta)} \binom{\alpha}{k} \binom{\beta}{k} \binom{2k}{\alpha+\beta-\lambda} \tag{B.15}$$

is the coefficient of $s^\alpha t^\beta$ in the power series expansion of $(1-st)^{-1} (1-a(s, t)^{-1})^2$. Using

$$\int_0^\infty \frac{e^{-u}}{x^2+u} du = e^{x^2} E_1(x^2) \tag{B.16}$$

and

$$(-1)^\lambda \int_0^\infty \frac{e^{-u}}{(x^2+u)^{\lambda+1}} du = \frac{1}{\lambda!} \sum_{k=1}^\lambda \frac{(-1)^k k!}{x^{2k}} + \frac{1}{\lambda!} e^{x^2} E_1(x^2) \tag{B.17}$$

for $\lambda \geq 1$, one can write (B.14) as

$$F_{\alpha\beta}(x) = \left[\sum_{\lambda=|\alpha-\beta|}^{\alpha+\beta} C_{\alpha\beta\lambda} x^{2\lambda} \right] e^{x^2} E_1(x^2) + \sum_{\nu=1}^{\alpha+\beta} D_{\alpha\beta\nu} x^{2(\nu-1)}, \tag{B.18}$$

with

$$C_{\alpha\beta\lambda} = \frac{(-1)^\lambda}{\lambda!} A_{\alpha\beta\lambda} \tag{B.19}$$

and

$$D_{\alpha\beta\nu} = (-1)^\nu \sum_{\lambda=1+\nu}^{\alpha+\beta} (-1)^\lambda (\lambda-1-\nu)! C_{\alpha\beta\lambda}. \tag{B.20}$$

By writing $F_{\alpha\beta}^{(1)}$ in the form

$$F_{\alpha\beta}^{(1)}(x) = g_{\alpha\beta}(x) e^{x^2} E_1(x^2) + h_{\alpha\beta}(x), \tag{B.21}$$

equating the derivative with (B.18), and solving the resulting differential equations for $g_{\alpha\beta}$ and $h_{\alpha\beta}$, one obtains

$$F_{\alpha\beta}^{(1)}(x) = x \left[\sum_{\lambda=0}^{\alpha+\beta} \frac{C_{\alpha\beta\lambda} x^{2\lambda}}{2\lambda+1} {}_1F_1 \left(1; \frac{3}{2} + \lambda; -x^2 \right) \right] e^{x^2} E_1(x^2) \\ + 2x \sum_{\lambda=0}^{\alpha+\beta} \frac{C_{\alpha\beta\lambda} x^{2\lambda}}{(2\lambda+1)^2} {}_2F_2 \left(1, \frac{1}{2} + \lambda; \frac{3}{2} + \lambda, \frac{3}{2} + \lambda; -x^2 \right) \\ + x \sum_{\nu=0}^{\alpha+\beta-1} \frac{D_{\alpha\beta\nu} x^{2\nu}}{2\nu+1}, \quad (\text{B.22})$$

where ${}_1F_1$ and ${}_2F_2$ are generalized hypergeometric functions [52]. In the same way one obtains the following expression for $F_{\alpha\beta}^{(2)}$:

$$F_{\alpha\beta}^{(2)}(x) = x^2 \left[\sum_{\lambda=0}^{\alpha+\beta} \frac{C_{\alpha\beta\lambda} x^{2\lambda}}{(2\lambda+1)(2\lambda+2)} \right. \\ \times {}_2F_2 \left(\frac{1}{2} + \lambda, 1 + \lambda; \frac{3}{2} + \lambda, 2 + \lambda; -x^2 \right) \left. E_1(x^2) \right] \\ + 2x^2 \sum_{\lambda=0}^{\alpha+\beta} \frac{C_{\alpha\beta\lambda} x^{2\lambda}}{(2\lambda+1)^2} {}_2F_2 \left(1, \frac{1}{2} + \lambda; \frac{3}{2} + \lambda, \frac{3}{2} + \lambda; -x^2 \right) \\ - 2x^2 \sum_{\lambda=0}^{\alpha+\beta} \frac{C_{\alpha\beta\lambda} x^{2\lambda}}{(2\lambda+2)^2} {}_2F_2(1, 1 + \lambda; 2 + \lambda, 2 + \lambda; -x^2) \\ + x^2 \sum_{\nu=0}^{\alpha+\beta-1} \frac{D_{\alpha\beta\nu} x^{2\nu}}{(2\nu+1)(2\nu+2)}. \quad (\text{B.23})$$

In Figs. 9, 10, and 11 we show the functions $F_{\alpha\beta}^{(1)}$, $F_{\alpha\beta}^{(2)}$, and $F_{\alpha\beta}^{(2)}$ for the lowest values of α and β .

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Note added in proof. TF and TFW theory for atoms in a magnetic field of arbitrary strength has previously been developed in a slightly different way from ours in [53]–[55]. An interesting point made in these papers is that the TF atom in a magnetic field has a finite radius.

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