

## Properties of the electron gas in a magnetic field and their implications for Thomas–Fermi type theories of matter

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We discuss the energy density of the homogeneous three-dimensional electron gas in a magnetic field in the Hartree–Fock approximation and demonstrate that it exhibits a series of first-order phase transitions when new Landau levels begin to be populated. We investigate consequences of this behavior for Thomas–Fermi type theories of matter in magnetic fields, and show that within this approximation it leads to singular features in electron density profiles.

The properties of matter in high magnetic fields are of interest both in the laboratory as well as in astrophysical contexts, where magnetic fields can be as high as  $10^{12}$ – $10^{13}$  G at the surfaces of neutron stars. We shall consider matter consisting of nuclei and non-relativistic electrons, since this is the case of interest at the relatively low densities ( $\leq 10^6$  g cm<sup>-3</sup>) at which the magnetic field affects the properties of matter appreciably. In the past a variety of theoretical methods have been used to calculate the properties of such matter [1–3]. Among these are two statistical models of matter, the Thomas–Fermi (TF) method, and the Thomas–Fermi method with exchange, the so-called Thomas–Fermi–Dirac (TFD) method. These methods have the virtue of simplicity, and in the absence of magnetic fields they have been shown to be asymptotically exact in the limit of infinitely large atomic numbers [4,5]. Previous application of these methods to matter in a magnetic field has been confined to the case of fields so high that only the lowest Landau level is occupied [3]. In this Letter we discuss general properties of these theories, and show that qualitatively new effects arise when electrons occupy more than the lowest Landau level.

The basic ingredients in the TF and TFD methods

are the energy densities of the spatially homogeneous electron gas treated as a free gas or in the Hartree–Fock (HF) approximation, and we begin by discussing them. The energy levels of a non-relativistic free electron in a magnetic field are given by

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

where  $\alpha$  is a non-negative integer specifying the Landau level,  $\sigma$  is the spin,  $p$  is the momentum along the field,  $m$  is the electron mass, and  $\omega_B = |e|B/mc$  is the cyclotron frequency. For a non-interacting electron gas in its ground state, new bands specified by the quantum numbers  $\alpha$  and  $\sigma$  begin to be filled at certain threshold densities  $n_{\alpha\sigma}^*$ . For densities slightly greater than a threshold density, added electrons go primarily into the newly occupied band, because its density of states has a one-dimensional character, and is therefore singular at low kinetic energies. As a consequence the compressibility of the electron gas behaves as  $1/(n - n_{\alpha\sigma}^*)$  for  $n$  just above  $n_{\alpha\sigma}^*$ . This physics is essentially the same as that which gives rise to the de Haas–van Alphen effect.

We next consider the effect of the exchange part of the interaction in the Hartree–Fock approximation. The effect of the long-range part of the Coulomb in-

teraction is assumed to be compensated by a uniform neutralizing background of positive charge. In TF and TFD theories it is assumed that locally the energy density is given by that for a homogeneous electron gas. We must therefore take the basic electron states to be plane waves, and consequently inhomogeneous ground states, such as charge density waves and Wigner crystals [6], play no role here. The sum of the kinetic and exchange energy densities of a homogeneous electron gas may be written in the form

$$w = \sum_{p\alpha\sigma} \left( \frac{p^2}{2m} + (\alpha + \frac{1}{2} + \sigma)\hbar\omega_B \right) n_{p\alpha\sigma} - \frac{1}{2} \sum_{pp'\alpha\beta\sigma} V_{\alpha\beta}(p-p') n_{p\alpha\sigma} n_{p'\beta\sigma}, \quad (2)$$

where  $n_{p\alpha\sigma}$  is the total density of electrons with quantum numbers  $p$ ,  $\alpha$ , and  $\sigma$ . Since the Coulomb interaction leaves an electron's spin unaltered, the summation in the second term of eq. (2) is taken only over the common spin,  $\sigma$ . The single particle energy levels in a magnetic field are degenerate, and are characterized by  $p$ ,  $\alpha$ ,  $\sigma$ , and an additional quantum number,  $M$ , a possible choice for which is the angular momentum about the direction of the field, and  $n_{p\alpha\sigma}$  is the density of electrons with all allowed values of  $M$  but given values of  $p$ ,  $\alpha$  and  $\sigma$ . Since the density per unit area of states of different  $M$  is  $(2\pi a_H^2)^{-1}$ , where  $a_H = (\hbar c/|e|B)^{1/2}$  is the magnetic length, it follows that  $n_{p\alpha\sigma} = f_{p\alpha\sigma}/2\pi a_H^2 L$ , where  $f_{p\alpha\sigma}$  is the occupation number of a single state, and  $L$  is the normalization length in the direction of the field. As we explain in more detail elsewhere [7], the effective exchange energy summed over allowed  $M$  values is given by

$$V_{\alpha\beta}(q) = 2\pi \int_0^\infty \rho d\rho \int_{-\infty}^\infty dz e^{-y} L_\alpha(y) L_\beta(y) \times \frac{e^2}{(\rho^2 + z^2)^{1/2}} e^{-iqz/\hbar}, \quad (3)$$

where  $L_\alpha$  is a Laguerre polynomial and  $y = \rho^2/2a_H^2$ . For  $\alpha = \beta = 0$  this expression is equivalent to that of Danz and Glasser [8]. From eq. (2), one can obtain the quasiparticle energy  $\epsilon_{p\alpha\sigma} = \delta w / \delta n_{p\alpha\sigma}$ , and the effective mass,  $m_{p\alpha\sigma}^*$ , given by  $\partial \epsilon_{p\alpha\sigma} / \partial p = p / m_{p\alpha\sigma}^*$ . One finds

$$\frac{1}{m_{p\alpha\sigma}^*} = \frac{1}{m} + \frac{1}{(2\pi)^2 \hbar a_H^2 p} \times \sum_{\beta} [V_{\alpha\beta}(p - p_{F\beta\sigma}) - V_{\alpha\beta}(p + p_{F\beta\sigma})]. \quad (4)$$

Here  $p_{F\beta\sigma}$  is the Fermi momentum of a band, given by  $p_{F\beta\sigma} = 2\pi^2 \hbar a_H^2 n_{\beta\sigma}$ , where  $n_{\beta\sigma} = \sum_p n_{p\beta\sigma}$  is the total density of electrons in a band. For small  $q$ ,  $V_{\alpha\beta}(q)$  diverges as  $2\pi a_H^2 e^2 \ln(\hbar/q a_H)$  for  $\alpha = \beta$  and therefore the effective mass varies as  $1/\ln(|p - p_{F\alpha\sigma}|^{-1})$  for  $p$  close to the Fermi momentum of the band. In a magnetic field the low temperature specific heat of the electron gas in the Hartree-Fock approximation therefore behaves as  $T/\ln(T^{-1})$ , as it does in zero field [9].

The equilibrium populations of bands are determined by equating the chemical potentials. Thus, since the exchange energy is spin-dependent, the degeneracy between states in the  $\alpha$ th Landau level with  $\sigma = -\frac{1}{2}$  and the  $(\alpha - 1)$ th with  $\sigma = \frac{1}{2}$  is broken. This leads to a splitting of the threshold densities, and to a spin dependence of the effective mass and the cyclotron frequency. An additional effect of the exchange interaction is that the cyclotron frequency depends on the Landau index  $\alpha$ , and consequently oscillatory contributions to the thermodynamic functions will not be periodic in  $1/B$ .

Next we demonstrate that in the Hartree-Fock approximation the electron gas has a negative compressibility when the density of electrons in a band is small. We investigate stability by calculating the second derivative of the energy density with respect to the populations of the bands. One finds

$$\frac{\partial^2 w}{\partial n_{\alpha\sigma} \partial n_{\beta\sigma'}} = \frac{\partial \mu_{\alpha\sigma}}{\partial n_{\beta\sigma'}} = \delta_{\alpha\alpha'} \left( \frac{2\pi^2 \hbar a_H^2 p_{F\alpha\sigma}}{m_{pF\alpha\sigma}^*} \delta_{\alpha\beta} - \frac{1}{2} [V_{\alpha\beta}(p_{F\alpha\sigma} + p_{F\beta\sigma}) + V_{\alpha\beta}(p_{F\alpha\sigma} - p_{F\beta\sigma})] \right). \quad (5)$$

Here  $\mu_{\alpha\sigma}$  is the chemical potential of electrons in Landau orbital  $\alpha$  and with spin  $\sigma$ . We note that  $\partial^2 w / \partial n_{\alpha\sigma} \partial n_{\beta\sigma'}$  is well defined for  $\alpha = \beta$  because the divergent term  $V_{\alpha\beta}(p_{F\alpha\sigma} - p_{F\beta\sigma})$  in eq. (5) is cancelled by an equal and opposite contribution to  $m_{pF\alpha\sigma}^*$ , and it may be written as  $\delta_{\sigma\sigma'} [2\pi^2 \hbar a_H^2 p_{F\alpha\sigma} / \tilde{m}_{pF\alpha\sigma}^* - V_{\alpha\alpha}(2p_{F\alpha\sigma})]$ , where  $\tilde{m}_{pF\alpha\sigma}^*$  is given by eq. (4), but



without the term for  $\beta = \alpha$ . The results for  $m^*$  and  $\partial^2 w / \partial n_{\alpha\sigma} \partial n_{\beta\sigma}$  are analogous to the corresponding results for a three-dimensional Fermi liquid [10], except that discrete sums over parallel and antiparallel relative orientations of momenta appear in the present one-dimensional case instead of integrals over angles between quasiparticle momenta.

Let us now examine the second derivative (5) for  $\alpha = \beta$ . In the absence of the exchange interaction this tends to zero as  $n_{\alpha\sigma} \rightarrow 0$  from above, since  $p_{F\alpha\sigma} \sim n_{\alpha\sigma}$ . On the other hand,  $V_{\alpha\alpha}(2p_{F\alpha\sigma})$  is positive definite and diverges logarithmically. Thus  $\partial^2 w / \partial n_{\alpha\sigma}^2$  is negative in the vicinity of  $n_{\alpha\sigma} = 0$ . This behavior is suggestive of a thermodynamic instability. More detailed investigations [7] show that at a given density there can be multiple solutions of the HF equations. One finds that in the state with lowest energy density for given electron density, the population of a band is not a continuous function of the total density; rather it increases discontinuously from zero to a finite value at the density  $n_c$  (depending on the band) at which the energies of the two lowest energy solutions of the HF equations cross. The chemical potential drops discontinuously at  $n = n_c$ , which implies that  $w$  is not a convex function of  $n$  in the neighborhood of  $n_c$ . We emphasize that this property does not hinge on the logarithmic singularity of the matrix element for small  $p = 2p_{F\alpha\sigma}$ . This singularity disappears when screening is taken into account, but provided the effective exchange interaction is positive and nonzero as  $p \rightarrow 0$ ,  $w$  will not be convex.

We now turn to the application of the above results to Thomas-Fermi theory, which is an approximate method for determining the properties of a system of nuclei (usually considered as point charges  $Z_i e$  at fixed positions,  $X_i$ ) and electrons which are assumed to form a gas with density  $n = n(x)$ , where  $x$  is the position. The TF ground state energy of a neutral system is given by the infimum of the so-called TF energy functional of  $n$ , subject to the condition that the total electronic charge equals the charge of the nuclei. The corresponding variational equation for the electron density is the TF equation

$$\begin{aligned} w'[n(x)] - e\Phi(x) - \lambda &= 0, & \text{if } n(x) > 0, \\ &\geq 0, & \text{if } n(x) = 0. \end{aligned} \quad (6)$$

Here the prime denotes differentiation with respect

to  $n$ ,  $w$  is the kinetic part of the electronic energy density (in TF theory) or the sum of the kinetic energy density and the exchange energy density (in TFD theory),  $\Phi(x)$  is the total electrostatic potential due to both nuclei and electrons, and  $\lambda$  is a constant, which is equal to the total electrochemical potential of the electrons. In TFD theory, the function  $w(n)$  is given by expression (2) evaluated for those electron densities  $n_{p\alpha\sigma}$  in the individual bands that minimize the energy (2) for a given total density  $n = \sum_{p\alpha\sigma} n_{p\alpha\sigma}$ .

As discussed by Lieb [5] the TF equation has a unique solution provided the energy density,  $w$ , satisfies the following conditions:

(i)  $w$  is continuously differentiable, convex and  $w(0) = 0$ .

(ii) For large  $n$ ,  $w'(n) \geq cn^{1/2+\epsilon}$ , where  $c$  and  $\epsilon > 0$ .

(iii) For small  $n$ ,  $w'(n) \leq w'(0) + c'n^{1/3+\epsilon}$ , where  $c' < \infty$  and  $\epsilon > 0$ .

More generally, it is in fact sufficient to require (i)-(iii) for the *convex hull* of the energy density,

$$w^*(x) := \sup\{l(x) \mid l(y) = ay + b, l(y) \leq w(y)\}. \quad (7)$$

The existence and uniqueness of a solution of the TF equation thus depends only on the behavior of  $w^*$  at low and high electron densities.

The basic reason for this is that the solution of the TF equation with energy density  $w^*$  does not take on values in intervals where  $w^*$  is different from  $w$  (ref. [11], cf. ref. [5], theorem 3.19). This last result can be understood as follows: Since the compressibility  $\kappa = [n^2 w^{*''}(n)]^{-1}$  diverges for densities where  $w^*$  is not strictly convex, it is clear that such densities can only occur in regions where the local pressure  $P = n w^{*'}(n) - w^*(n)$  is strictly constant. In such regions the electrostatic potential  $\Phi$  must also be constant by the equation of hydrostatic equilibrium,  $\nabla P = en \nabla \Phi$ , which follows from the TF equation (6). This, however, contradicts the Poisson equation  $\nabla^2 \Phi(x) = 4\pi e [n(x) - \sum_i Z_i \delta(x - X_i)]$  for  $n(x) > 0$ . We note in passing that the argument remains true even if the positive charge has a continuous distribution, as long as the positive charge density avoids intervals where  $w^*$  is not strictly convex.

From this result it follows (cf. ref. [5], theorem 6.8, and ref. [7]) that the TF equation with energy

function  $w$  has exactly the same solution as the equation with energy function  $w^*$ . In particular this solution does not take on values in density intervals where  $w$  is not strictly convex. Thus for the energy function such as the one shown in fig. 1, the solution of the TF equation does not take on values for the electron density less than  $n^{(0)}$  or in the interval  $(n^{(1)}, n^{(2)})$ . A TF calculation for an isolated atom with this  $w$  would show a density profile as pictured schematically in fig. 2. The density jump at the atomic edge arises because the pressure  $P$  vanishes for  $n < n^{(0)}$ , while the absence of densities between  $n^{(1)}$  and  $n^{(2)}$  means that the two phases with densities

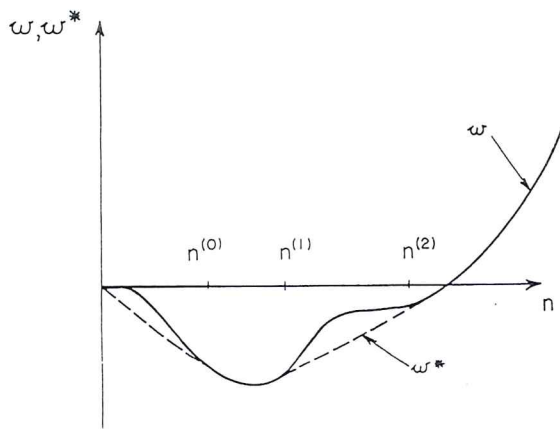


Fig. 1. Schematic sketch of an energy density,  $w$ , and its convex hull,  $w^*$ .

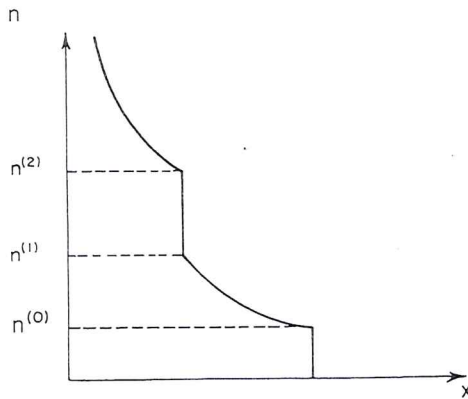


Fig. 2. Schematic sketch of the electron density in an atom in the Thomas-Fermi-Dirac approximation for the energy function shown in fig. 1.

$n^{(1)}$  and  $n^{(2)}$  are in equilibrium. For  $n^{(1)} \leq n \leq n^{(2)}$ , the function  $w^*$  is obtained from  $w$  by making a double tangent construction, so  $P(n^{(1)}) = P(n^{(2)})$  and  $\mu(n^{(1)}) = \mu(n^{(2)})$ , which are the usual thermodynamic conditions for phase equilibrium.

As we described above, in the Hartree-Fock approximation the energy density of the electron gas in a magnetic field displays an infinite number of density intervals where  $w$  is not a convex function of  $n$ . In TFD theory this leads to jumps in electronic density profiles of the type illustrated in fig. 2. As we shall show elsewhere [7], the characteristic size of the density jumps in strong fields is determined by the small parameter  $a_H/a_0$ , where  $a_0$  is the Bohr radius, which is a measure of the ratio of the exchange energy to a typical kinetic energy.

In TF theory in a magnetic field  $w''$  vanishes only at isolated points, but even this will have qualitative effects on the behaviour of  $n(x)$ . For example, in the spherically symmetric case considered above one has  $w''(n(r))dn/dr = dw'(n(r))/dr = ed\Phi(r)/dr$  by the TF equation, so  $dn/dr = [w''(n(r))]^{-1} d\Phi(r)/dr$  diverges if  $w''$  approaches zero. This remark applies to the kinetic part of the energy functional (2), when  $n$  approaches a threshold density from above.

Finally we consider possible molecular binding of atoms in high magnetic fields. For the case of zero field, it has been shown that in TF and TFD theory there is no binding, that is, the energy will always decrease if the nuclei are separated into two or more groups, and groups are moved far away from each other. Thus, while these theories are useful for describing the main features of electronic densities and ground state energies, they are unsuitable for computing effects as delicate as molecular binding. Teller [12] investigated this question in the standard TF and TFD approximations in which the kinetic energy is proportional to  $n^{5/3}$ , and the exchange energy is negative and proportional to  $n^{4/3}$ . The paper by Lieb, Simon, and Benguria [4,5,11] are also concerned mainly with these special forms of  $w$ . However, their extension of Teller's work is quite general, and it follows from theorem 3.23 of ref. [5] that binding does not occur for any  $w$  satisfying conditions (i)-(iii) given above. This is also obvious from the proof given in ref. [13] for  $w(n) = \text{const} \times n^{5/3}$ ; granted existence of a solution of (6), the only special property of this function used is its convexity.



But, as remarked above, the TF energies calculated with an arbitrary  $w$  are the same as those calculated with its convex hull,  $w^*$ . Thus TF theory is well defined and the no-binding theorem holds for any  $w$ , provided its convex hull satisfies conditions (i)–(iii) above. This is indeed the case for the energy densities considered above: For large  $n$ , the effects of the magnetic field and exchange energy become negligible and therefore  $w^* \sim cn^{5/3}$ . For small  $n$ ,  $w^{*'} < c' n^2$  in the absence of the exchange term where  $c$  and  $c'$  are constants, and  $w^{*'}$  is a negative constant if the exchange energy is included.

In this paper we have restricted our attention to theories of the Thomas–Fermi type in which the electronic energy density at a given point depends only on the value of the electronic density at the same point. More generally, one can consider theories where non-local effects are taken into account by, for example, including a von Weizsäcker term, which depends on the gradient of the electron density. In such theories the density jumps found in theories with local energy functionals will tend to be smoothed out. These effects will be studied in more detail elsewhere [7].

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