Statistical Model of Atoms in Intense Magnetic Fields*

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(Received 11 March 1971)

We obtain the dimensions R, electron density distributions $n(\vec{r})$, and total ground-state binding energies E of atoms and positive ions (nuclear charge Z, N electrons) in intense magnetic fields. A variationally formulated Thomas-Fermi–like model is valid for $Z^{4/3} \ll 10^{-9}B \ll 10Z^3$ G; the choice $n(\vec{r}) \sim ZR^{-3}\sigma^{-1/4}\exp(-\sigma)$, $\sigma \equiv r^2/R^2$, gives $E \approx -150(B/10^{12})^{2/5}Z^{9/5}$ eV, for neutral atoms. A crude variational calculation, valid for $B \gg 10^{10}Z^3$, gives $E \approx -13.6N(Z-\frac{1}{3}N)^2\ln^2(2B/10^{10})$ eV.

The determination of the properties of atoms and ions in an intense magnetic field[1-3] $\vec{B}$ has assumed added importance with the discovery of pulsars. We will be primarily concerned with the regime within which a "one-dimensional" statistical model is adequate, particularly for the determination of ground-state energies.

Throughout, we restrict ourselves to a uniform intense magnetic field $\vec{B}$, taken to be parallel to the z axis. For an electron in a field $\vec{B}$, the motion in the ρ, φ plane perpendicular to $\vec{B}$ is described by the Landau-level wave functions $\psi_{nm}(\rho, \varphi)$. The (infinitely degenerate) ground-state functions are given by $\psi_{0m} \sim R_m(\rho)\exp(im\varphi)$, where $R_m(\rho) \sim q^{|m|}\exp(-\frac{1}{2}q^2)$ with $q \equiv \rho/\hat{\rho}$, $\hat{\rho}^2 \equiv 2c\hbar/eB$, and $m = 0, -1, -2, \cdots$. The energy separation between this level and the next is given by $\Delta E = eB\hbar/\mu c$, where μ is the electron mass. For an atom or ion with nuclear charge Z and N electrons, B will be called intense if ΔE is so large that the Coulomb forces do not excite the electrons from the ψ_{0m} states (though they do determine the distribution among these states). The electrons are tied to the magnetic lines of force; the Coulomb field contains the electrons with respect to their z motion.

Consider for the moment a single electron interacting with the nucleus in the presence of the field $\vec{B}$. The effective one-dimensional potential seen by an electron with quantum number m, obtained by integrating Ze/r over $R_m^2(\rho)$, is given roughly for $|m| \gg 1$ by $Ze/(z^2+\hat{\rho}_m^2)^{1/2}$, where $\hat{\rho}_m \equiv \hat{\rho}\,|m|^{1/2}$ is the value of ρ at which R_m^2 is sharply peaked. This in turn is approximated (and bounded) by $Ze/(|z|+\hat{\rho}_m)$. The energy spectrum for this latter potential is known[4] for the ρ dimension of the orbit much smaller than the z dimension, that is, for $\hat{\rho}_m \ll a_0/Z$ ($a_0 = \hbar^2/\mu e^2$). For fixed m this will be the case for B sufficiently large. The spectrum includes eigenvalues close to the Bohr levels associated with Ze/r; in addition, it includes one (and only one) eigenvalue much below the lowest Bohr value, $-Z^2E_H$ ($E_H = 13.6$ eV), given approximately by $E_{deep} = -4E_HZ^2\ln^2(a_0/Z\hat{\rho}_m)$. It is useful to define m_{max} as the absolute value of that m for which the ρ and z dimensions are comparable, that is, for which $\hat{\rho}_m = a_0/Z$. For $\hat{\rho}_m \gg a_0/Z$, that is, for $|m| \gg m_{max}$, all of the eigenvalues, including the "deep" level, lie much above $-Z^2E_H$.

It is important to subdivide intense fields into what we shall call "ultrastrong" and "strong" fields. For *ultrastrong* fields, one has $m_{max} \gg N$, and all electrons can take full advantage of the deep level states; the ground-state wave function Ω is well approximated by $\mathcal{A}\prod\psi_{0m}(\rho, \varphi)g_m(z)$, where $\mathcal{A}$ is the antisymmetrization operator, the nodeless functions g_m are those associated with E_{deep}, and there are N different values of m. [The values of m may not be 0, -1, -2, $\cdots$, $-(N-1)$; it is preferable to introduce gaps if the reduction in absolute magnitude of the energy of attraction of the electrons by the nucleus is more than compensated for by the reduction of the electron-electron energy of repulsion.[1]] For *strong* fields, one has $m_{max} \ll N$. States with values $|m| \gg m_{max}$ are much less bound than the lower Bohr levels, and one then expects only states with $|m| \ll N$ to be occupied in the ground state; there are a number $\nu(m)$ of electrons associated with each such m, and the associated functions of z have from zero up to $\nu(m)-1$ nodes. It is then possible to ascribe a meaningful estimate to the value of p_z, the z component of momentum, and it may therefore be possible to use a "one-dimensional" statistical model for the strong field case.

Estimates of the total binding energies of atoms and ions have not previously been given, but for light atoms and $B = 2.2\times10^{12}$ G—this will be seen later to represent roughly the overlap region between strong and ultrastrong fields—the binding energy of the last electron was obtained.[2] Reliable estimates of the binding energy of the

last electron, which may play a role in the determination of the probability of the associated ion being accelerated by the strong electric fields near a pulsar, cannot be obtained in the statistical model to be considered.

Atoms in strong magnetic fields have also been studied.[1] This case, our primary concern, was formulated in terms of a differential equation which is the analog of that obtained in the Thomas-Fermi (TF) approach. The limits of validity of the TF-like approach were obtained, as was the dependence of the dimension R of the atom on B and Z. The approach contains an approximation which does not seem to us to have been fully justified, namely, the number density of electrons $n(\vec{r})$ is not restricted to be a superposition of the Landau $|\psi_{0m}|^2$. (This "ground-state restriction" cannot be imposed in the differential-equation approach.) The approach is made somewhat self-consistent by the requirement that the results obtained be accepted only if the TF-like potential $\varphi(\vec{r})$ calculated is too weak to excite higher Landau levels, but one might imagine the unrestricted $n(\vec{r})$ to give binding energies off by a significant factor even for $e\varphi(\vec{r})$ small compared to ΔE for most r. ($e>0$ is the magnitude of the charge of the electron.) We will show that use of the unrestricted $n(\vec{r})$ is entirely justified in the domain of validity of the statistical model.

We also use a statistical or TF-like model for the strong-field case, but we use a variational[5] rather than differential-equation formulation. The ground-state restriction on $n(\vec{r})$ is then readily incorporated. Ions and atoms can then be treated on the same basis[5] (though not necessarily to the same degree of accuracy), that is, one calculation suffices for all atoms and ions. (It would be trivial to extend the approach to high-density situations in which an atom is confined to a given volume, as, for example, in the outer layers of the crust of a pulsar.) Further, the calculation is not numerical; one can easily obtain an analytic approximation to $n(\vec{r})$ which is sufficiently simple and accurate to enable one to compute reliably certain atomic and ionic properties. We will use the analytic $n(\vec{r})$ only to calculate the ground-state energy $E_{str}=E_{str}(Z,N,B)$.

To perform the calculation, we need the connection between the kinetic energy and $n(\vec{r})$. We note that the number of (otherwise free) electrons per unit volume in a uniform field B with momentum between p_z and p_z+dp_z is[6] $K\theta(p_z)dp_z$, where $K\equiv eB/h^2c$, $p_F=p_F(\vec{r})$ is the Fermi momentum, and $\theta(p_z)=1$ for $|p_z|<p_F$ and $\theta(p_z)=0$ for $|p_z|>p_F$. It immediately follows that $n(\vec{r})=2Kp_F(\vec{r})$. (Note that all electron spins are assumed to be antiparallel to $\vec{B}$.) Let T_z be the kinetic energy associated with motion parallel to $\vec{B}$. [Both the kinetic (or magnetic) energy associated with motion in the ρ-φ plane and the energy of alignment of the electron magnetic moments with respect to $\vec{B}$ are assumed to be unperturbed by the Coulomb fields, and their sum serves as our zero-energy reference level.] T_z is given by

$$T_z=\int d^3r\int(p_z^2/2\mu)K\theta(p_z)dp_z$$
$$=e^2L^5\int n^3(\vec{r})\,d^3r, \qquad (1)$$

where $L^5\equiv\pi^4a_0\hat{\rho}^4/6$. $E_{str}=T_z+V_{en}+V_{ee}$ then becomes

$$E_{str}=e^2\{L^5\int n^3\,d^3r-Z\int nr^{-1}d^3r$$
$$+\tfrac{1}{2}\int\int n(\vec{r})n(\vec{r}')s\,d^3r\,d^3r'\}, \qquad (2)$$

where $s\equiv|\vec{r}-\vec{r}'|^{-1}$ and the subscripts e and n refer to the electron and nucleus, respectively. [The exchange contribution has been lost by the use of $n(\vec{r})$ rather than the correct wave-function description. An estimate of the exchange term can be obtained,[7] in terms of $n(\vec{r})$, but it is of lower order in Z than the direct term and will be ignored.]

The objective now is to minimize $E_{str}=E_{str}(n(\vec{r}))$ with respect to parameters contained in an $n(\vec{r})$ which must satisfy the obvious conditions that (i) $n(\vec{r})\geq 0$ for all r, and (ii) $\int n(\vec{r})\,d^3r=N$. The ground-state restriction requires that the form of $n(\vec{r})$ be (iii) $n(\vec{r})=\sum_m R_m^2(\rho)f_m^2(z)$, where the $f_m(z)$ are arbitrary. A further condition, obtained from energy considerations,[8] is that $n(\vec{r})$ be spherically symmetric. It then follows[8] that $n(\vec{r})=n(r^2)$. We can now extract the dependence of the dimension R and the energy E_{str} on Z, N, and B. Since only one length, L, is present, we can always write $n(\vec{r})=NR^{-3}n^*(x^2)$, where $x\equiv r/R$, $n^*(x^2)\geq 0$ for all x, and $\int n^*(x^2)dx=1$. (R will be proportional to L.) This satisfies all of the necessary conditions, and we have

$$E_{str}=e^2N\{t_zN^2(L/R)^5-Zv\}R^{-1},$$

where $v\equiv v_{en}-v_{ee}NZ^{-1}$, and where t_z, v_{en}, and v_{ee} are dimensionless positive numbers independent of Z, N, and B; further, we have $v_{en}>v_{ee}$, and, assuming as we always will that $N\leq Z$, we have $v>0$. The minimum value of E_{str}, obtained for $R/L=(6t_zN^2/Zv)^{6/5}$, is $E_{str}=-5t_z^{-1/5}\times N^{3/5}(\frac{1}{6}Zv)^{6/5}e^2/L$. [Notice that $3T_z=-\frac{1}{2}(V_{en}$

$+V_{ee}$), which is just the virial theorem for a spherical distribution of charged particles.[9]] v is roughly independent of Z and N since $v_{ee}N \times Z^{-1}$ is small compared to v_{en} (see later) and we then have, roughly, $R \sim (N^2/ZB^2)^{1/5}$ and $E_{str} \sim (N^3Z^6B^2)^{1/5}$. For neutral atoms ($N=Z$), v is strictly independent of Z and N and we have exactly, within the framework of the model, $R \sim B^{-2/5}Z^{1/5}$ and $E_{str} \sim B^{2/5}Z^{9/5}$. These scaling properties are to be contrasted with the usual TF results, $R \sim Z^{-1/3}$ and $E_{TF} \sim Z^{7/3}$.

A necessary and sufficient condition for any function to satisfy the ground-state restriction is that it be a function of r^2 and fall off slower than $\exp(-r^2/\hat{\rho}^2)$.[8] Since $n(r^2)$ can therefore be arbitrary, variation of $n(r^2)$ in (2) gives, in the usual way,

$$3L^5e^2n^2(r) = Ze^2/r - e^2\int n(r')\,|\vec{\mathbf{r}}-\vec{\mathbf{r}}'|^{-1}d^3r - e\varphi_0; \quad (3)$$

φ_0 is a Lagrange undetermined multiplier. This is the standard TF relation, $p_F^2(r)/2\mu - e\varphi(r) = -e\varphi_0$, where $\varphi(r)$ is the total potential and φ_0 is a positive constant for ions[5] and zero for neutral atoms; we now have a firm justification for the TF-like differential-equation approach of Ref. 1.

A heuristic argument may be helpful. The most obvious possible extension of the standard TF relation for the spherically symmetric situation to the case of an external field B is $p_F^2(\rho,z)/2\mu - e\varphi(\rho,z) = -e\varphi_0(\rho)$, the electrons adjusting themselves, *for each value of* ρ (their freedom of motion in the ρ-φ plane is rather restricted) so that the maximum energy is the same. For the validity of the statistical model, however, we have seen that $n(r)$ must be spherically symmetric, as must also $p_F(r)$ and $\varphi(r)$. It is then clear, however, that φ_0 cannot be $\varphi_0(\rho)$ but must be a constant.

The $-Ze^2/r$ behavior of $-e\varphi(r)$ as $r \to 0$ requires $n(r)$ to have an $r^{-1/2}$ singularity as $r \to 0$. This is inconsistent with (iii)′ but the TF-like model is in any event invalid near $r=0$, and we will include this singularity in our choice of $n(r)$ simply to conform with the usual TF procedure[10] and since we believe that for r small but not too close to the origin the falloff of $n(r)$ is well described by $r^{-1/2}$. (The omission of the singularity scarcely alters the value of E_{str} we obtain and changes R by only 15%.) The simplest choice which satisfies all of the conditions is $n(r) = C(N/R^3)\exp(-x^2)x^{-1/2}$, where $x \equiv r/R$ and $C^{-1} = 2\pi\Gamma(\frac{5}{4})$. The minimum energy, achieved for $R \approx 7\times10^{-10}(N^2/ZB_{12}^2)^{1/5}\tau^{-1}$ cm, where B_{12} is B measured in units of 10^{12} G, is $E_{str} \approx -150 \times (N^3Z^6B_{12}^2)^{1/5}\tau^6$ eV, where $\tau \approx [\frac{3}{2}-\frac{1}{2}(N/Z)]^{1/5}$, and therefore $\tau = 1$ for the neutral atom. (This is to be contrasted with the usual TF result, $E_{TF} \approx -20Z^{7/3}$ eV.) The analytic $n(r)$ above agrees fairly well with that obtained numerically[1] for $N=Z$.

One relation between the numbers T_z, V_{en}, and V_{ee} has already been noted. A second relation follows in the same fashion as for the normal TF model.[11] V_{ee} of (1) can be written as $-\frac{1}{2}e\int n(r) \times \varphi_e(r)\,d^3r$, or, using (3), $2V_{ee} = -V_{en} - 3T_z - e\varphi_0 N$. Combining this relation with that obtained from the virial theorem, we find for the neutral atom, for which $\varphi_0 = 0$, that $V_{ee} = -\frac{1}{3}V_{en}$. The use of our analytic $n(r)$ gives $V_{ee} = -0.33\,V_{en}$.

We turn now to the range of validity of the statistical model, restricting ourselves for simplicity of discussion to $N=Z$. One would expect E_{str} to lie below the energy obtained by ignoring B and using the usual E_{TF} result. This gives $B \gg 10^9Z^{4/3}$ G. [An identical result is obtained if one makes the demand, commented on earlier, that $e\varphi(r)$ for all r but $r \approx 0$ be much less than the separation of the Landau levels.] To obtain an upper limit on B, we again note that the statistical model can be valid only if it is possible to define p_z. It is *not* possible to do so if all or many of the electrons lie in the deep-level states, states characterized by nodeless z-dependent functions. The condition for an electron not to be in such a level is $\hat{\rho}_m \gg a_0/Z$. Requiring at least that an electron with a large value of $|m|$, say $\frac{1}{2}Z$ (which sees an effective change of order $\frac{1}{2}Z$), not be in a deep level gives $B \ll 10^{10}Z^3$ G. A similar result is obtained on applying the usual validity criterion for the TF approximation, namely, $\varphi^{-1}(d\varphi/dr)^{\frac{1}{2}} \ll 1$. The statistical model therefore has a reasonably wide range of validity. For 10^{12} G, for example, it is roughly valid for $5 \lesssim Z \lesssim 50$. Note that we expect the statistical model to be valid even if a few electrons lie in deep levels.

We make only a few brief comments on the ultrastrong case. Simply ignoring V_{ee} gives a ground-state energy E_{ul} which is a sum over E_{deep} values, or, since the m dependence of the argument of the logarithm can be dropped without appreciable error for $a_0/Z \gg \hat{\rho}_m$, we have $E_{ul} \approx -4Z^2NE_H\ln^2(a_0/\hat{\rho}) \equiv -E'Z^2N$. Treating the electron-electron interaction as a perturbation (even though it is not all that small), with Ω as

the zero-order wave function, raises the energy to $E_{ul} \approx -E'Z(Z-\frac{2}{3}N)N$. A preliminary variational calculation improves this last result to $E_{ul} \approx -E' \times (Z-\frac{1}{3}N)^2N$. A possibility of gaps in filling in m states will surely change the numerical coefficient, but may well not affect the Z and B dependence of E_{ul}, which is qualitatively different from the B and Z dependence of E_{str}.

We would like to thank M. Ruderman for a number of very helpful conversations and L. Rosenberg for a useful remark.

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*Work supported by the U. S. Army Research Office, Durham, and by the Office of Naval Research.

†Submitted in partial fulfillment of the requirement for the degree of Doctor of Philosophy at New York University.

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[2]R. Cohen, J. Lodenquai, and M. Ruderman, Phys. Rev. Lett. 25, 467 (1970).

[3]See, however, R. G. Newton, Phys. Rev. D 3, 626 (1971). See also R. Barbieri, Nucl. Phys. A161, 1 (1971).

[4]L. K. Haines and D. R. Roberts, Amer. J. Phys. 37, 1145 (1968).

[5]For the variational TF model, see A. A. Sokolov, Y. M. Loskutov, and I. M. Ternov, *Quantum Mechanics* (Holt, Rinehart and Winston, New York, 1966), p. 400.

[6]L. D. Landau and E. M. Lifschitz, *Quantum Mechanics: Non-Relativistic Theory* (Addison-Wesley, Reading, Mass., 1965), 2nd ed., Sect. 111.

[7]J. C. Slater, *Quantum Theory of Matter* (McGraw-Hill, New York, 1951), Appendix 22.

[8]We write $n(\vec{r}) = n_0(r) + n'(\vec{r})$, where $n_0(r)$ is the average value of the non-negative $n(\vec{r})$ with respect to integration over angles and is therefore itself non-negative. Since the angle average of $n'(\vec{r})$ vanishes by definition, the difference between $E(n(\vec{r}))$ and $E(n_0(r))$ is given by $\delta = e^2L^5I + V_{ee}'$, where $I \equiv \int [3n_0(r) + n(\vec{r})] \times n'^2(\vec{r})\, d^3r$ is clearly non-negative. V_{ee}' is obtained from V_{ee} by the replacement of each n by n'. Using $t^{-1} \sim \int d^3k \exp(i\vec{k}\cdot\vec{t})/k^2$, where $\vec{t} \equiv \vec{r} - \vec{r}'$, we have that V_{ee}' is approximately the integral over k space of the square of the absolute magnitude of the Fourier transform of $n'(\vec{r})$. Since it is readily shown that for any $n(\vec{r})$ satisfying (iii) the associated $n_0(r)$ also satisfies (iii), and since (ii) is a condition on $n_0(r)$ only, it follows that $n(\vec{r}) = n(r)$. Combined with (iii) again, it can then be shown that (iii)' $n(r) = n(r^2)$. [Note that for $0 < \gamma < 1$, we have $\exp(-\gamma r^2/\hat{p}^2) \sim \sum R_m^2(\rho) \exp(-\alpha|m| - \gamma z^2/\hat{p}^2)$, where $\gamma = 1 - \exp(-\alpha)$, and $0 < \alpha < 1$.]

[9]The standard virial theorem, even in the presence of a magnetic field, gives $2T_z = z(\partial V/\partial z) = r(\partial V/\partial r)F$, $F \equiv 1 - \rho^2/r^2$, and averages understood. For a spherical distribution, $F = \frac{1}{3}$. For the ultrastrong regime, unless states with very high m are considered, $F = 1$.

[10]Attempts to improve the ordinary TF model by the omission of the corresponding (unphysical) $r^{-3/2}$ singularity have proved successful. See J. Goodisman, Phys. Rev. A 2, 1193 (1970).

[11]Section 70 of Ref. 6.

Fragmentation Models for Inelastic Lepton-Hadron Scattering*

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(Received 9 March 1971)

We propose models for deep inelastic lepton-hadron scatterings, incorporating the general ideas of the fragmentation picture. Approximate scaling behavior can be accommodated at present values of the momentum transfer. But at larger momentum transfers, significant deviations from scaling are expected. In contrast to the results of the parton model, a scaling behavior for the average multiplicity and the structure functions at fixed multiplicities is not possible, according to the fragmentation picture. We present results of our model regarding the average multiplicity and the structure functions.

One of the important features of the deep inelastic electron-scattering data[1,2] obtained at the Stanford Linear Accelerator Center (SLAC) is the approximate scaling behavior of the structure functions in the deep inelastic region, a feature first hypothesized by Bjorken.[3] This scaling property has been the focal point of many recent theoretical discussions. Inelastic muon-proton scattering experiments[4] are now being planned and are to be carried out at the National Accelerator Laboratory (NAL) at much higher energies than are presently available at SLAC. These experiments should be able to provide additional crucial tests of the scaling hypothesis and, moreover, yield valuable information about the more detailed properties of the final hadron