IC/2000/96

United Nations Educational Scientific and Cultural Organization
and
International Atomic Energy Agency

THE ABDUS SALAM INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS

A PROPOSED GENERALIZATION OF EMDEN'S DIFFERENTIAL EQUATION TO EMBRACE THE GROUND-STATE ELECTRONIC STRUCTURE OF EXTREMELY HEAVY POSITIVE ATOMIC IONS WITH AND WITHOUT APPLIED MAGNETIC FIELDS

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MIRAMARE – TRIESTE
August 2000

Abstract

The differential equation for the dimensionless screening function $\phi(x)$ of a point nucleus in an extremely heavy positive atomic ion is shown to have the form

$$\phi'' = \frac{\left\{\phi\left(1+\gamma\frac{\phi}{x}\right)\right\}^{n/2}}{x^{m/2}} \ .$$

This reduces to Emden's equation for $\gamma = 0$ and $m = n-2$. The above differential equation embraces four physical regimes: non-relativistic atomic ions with (i) magnetic field strength $B = 0$, (ii) B very large, cases (iii) and (iv) being the relativistic analogues of (i) and (ii). The pairs of n and m are restricted in regimes (i) - (iv) delineated above to $[3, 1]$ and $[1, -1]$. In the proposed differential equation above, γ is a dimensionless quantity. In zero magnetic field corresponding to $[n, m] = [3, 1]$, γ measures the ratio of a characteristic Coulomb energy Ze^2/b, with Z the atomic number of the ion and with b a scaling length $\propto Z^{-1/3}$, to the electron rest mass energy. γ involves also the magnetic field strength B in the intense magnetic field limit corresponding to $[n, m] = [1, -1]$.

1 Introduction and overview

Since the early work of Milne [1], it has been known that the study of the electronic structure of heavy atoms had mathematical content closely similar to previous investigations of Emden [2]. As summarized, for instance in the book by Saslaw [3], the problem of the structure of a gaseous star led Emden to a differential equation having the form

$$\frac{1}{x^2}\,\frac{d}{dx}\,\left(x^2\,\frac{d\theta}{dx}\right)+\theta^n=0\ . \tag{1.1}$$

n is known as the polytrope index and enters the 'effective equation of state' through the power law form $p=K\rho^{1+1/n}$.

Returning to Milne's study, he was concerned with the total ground-state energy of a heavy neutral atom of atomic number Z. Then a central quantity is the self-consistent potential energy $V(r)$ felt by an electron in the charge cloud surrounding the nucleus. In the limit of large Z, it is helpful to write [4]

$$V(r)=-\frac{Ze^2}{r}\,\phi(x):r=bx,\quad b=\frac{1}{4}\left(\frac{9\pi^2}{2}\right)^{1/3}\,\frac{a_0}{Z^{1/3}}: \tag{1.2}$$

where the 'screening function' $\phi(x)$ satisfies the differential equation [5-7]

$$\frac{d^2\phi}{dx^2}=\frac{\phi^{3/2}}{x^{1/2}}\ , \tag{1.3}$$

and a_0 is the Bohr radius. As Milne [1] noted, this differential eqn (1.3), apart from a sign, is a special case of Emden's eqn (1.1) with $n=\frac{3}{2}$ and $x\theta\equiv\phi$.

For neutral heavy atoms, the boundary conditions under which eqn (1.3) must be solved are evidently

$$\phi(x=0)=1 \tag{1.4}$$

and

$$\phi(x)\Big|_{x\to\infty}\to 0 \tag{1.5}$$

Sommerfeld [8] pointed out that $\phi=144/x^3$ was an exact solution of eqn (1.3), but satisfying the boundary condition (1.5) only, while Coulson and March [9] generated the asymptotic expansion for large x, namely

$$\phi(x)=\frac{144}{x^3}\,\left[1-\frac{F_1}{x^c}+\frac{F_2}{x^{2c}}+\ldots\right] \tag{1.6}$$

and tabulated the numbers f_n in $F_n = f_n(F_1)^n$ out to $n = 10$. The index c in eqn (1.6) has the interesting feature that it is irrational, having the value

$$c = \frac{\sqrt{73} - 7}{2} = 0.772 \ . \tag{1.7}$$

Such a situation, of course, is very familiar to workers in statistical mechanics. Though eqn (1.3) can describe neutral atoms, characterized by boundary condition (1.5), it is in fact the basic equation of the so-called Thomas-Fermi statistical theory of heavy positive atomic ions with atomic number Z and N electrons, with evidently then $N \leq Z$. This theory has a range of validity that requires both N and Z to be large, though one can still allow highly ionized configurations with $N/Z \ll 1$. Returning briefly to the solution (1.6), Coulson and March [9] showed that with the choice $F_1 = 13 \cdot 21$ it could be extended inwards (say by numerical integration) to satisfy the initial condition (1.4).

After this introduction, section 2 below will be concerned with a brief description of the way in which the introduction of Special Relativity modifies the above statistical method. Specifically, we shall build on the study of Hill, Grout and March [10], who obtained the counterpart of eqn (1.3) for relativistic heavy positive atomic ions in an intense magnetic field of strength B.

2 Differential equation for screening function $\phi(x)$ for relativistic atomic ions in an intense magnetic field

In the Thomas-Fermi theory summarized in the previous section, a basic equation is that for the chemical potential μ, which is constant throughout the entire inhomogeneous charge cloud of the atomic ions, having electron density $\rho(\underset{\sim}{r})$.

Let us now generalize this by invoking the Special Relativity relation between kinetic energy and momentum. Then, using the fine structure constant $\alpha = e^2/\hbar c$ to characterize the corresponding chemical potential, one has [10]

$$\mu_\alpha = \left\{ \frac{c^2 h^4}{4e^2 B^2} \ \rho^2(r) + m_0^2 c^4 \right\}^{1/2} - m_0 c^2 + V(r) \tag{2.1}$$

where the quantity $m_0 c^2$, the electron rest mass energy, has been subtracted from the relativistic kinetic energy represented by the first term on the RHS of eqn (2.1).

Rearranging eqn (2.1) and squaring yields, after a short calculation, the result

$$\frac{(\mu_\alpha - V(r))^2}{2m_0c^2} + (\mu_\alpha - V(r)) = \frac{h^4}{8e^2m_0}\ \frac{\rho^2(r)}{B^2} \tag{2.2}$$

Hill et al. [10], who first derived eqn (2.2), then again introduced a screening function $\phi(x)$ through

$$[\mu_\alpha - V(r)] = -\frac{Ze^2}{r}\ \phi(x) \tag{2.3}$$

where (compare eqn (1.2)) the length scale $r = b'x$ is redefined by

$$b' = \frac{1}{2}\left(\frac{\lambda}{2\pi}\right)^{-2/5}\ Z^{1/5}a_0\ , \tag{2.4}$$

while

$$\lambda = (\mu_B B/Ry)\ , \tag{2.5}$$

μ_B being the Bohr magneton. It was then shown [10] that $\phi(x)$ obeys the differential equation

$$\phi'' = x^{1/2}\left\{\phi\left(1+\gamma\frac{\phi}{x}\right)\right\}^{1/2}\ , \tag{2.6}$$

γ being given by

$$\gamma = \left(\frac{\lambda}{2\pi}\right)^{2/5}\ \alpha^2\ Z^{4/5} \tag{2.7}$$

in terms of the fine structure constant $\alpha = e^2/\hbar c$. Evidently in the non-relativistic limit corresponding to $\alpha \to 0$ or equivalently $c \to \infty$, the quantity γ defined in eqn (2.7) goes to zero and one obtains the limiting equation from eqn (2.6) as

$$\phi'' = (x\phi)^{1/2} \tag{2.8}$$

This eqn (2.8), as with eqn (1.3) is another special case of Emden's eqn (1.1) (apart from a sign again), this time with $n = 1/2$.

A final (more physical) comment is in order here relating to eqn (2.6) and its non-relativistic limit in eqn (2.8). It will have been noted that, even though these are equations valid in intense magnetic fields of strength B, the resulting screening function $\phi(x)$ is still spherically symmetrical. The physical understanding of such a situation has been clarified, for example, in the work of Lieb, Solovej and Yngvason [11], which is characterized by comparing the field strength B in suitable units with powers of atomic number Z. In fact these workers delineate five different regimes. Roughly speaking, they show that

B/Z^3 is playing the role of an effective Planck's constant, and it is only when $B \sim Z^3$ and $B \gg Z^3$ that in the heavy atom limit discussed above the screening departs from spherical symmetry. In the last region with B/Z^3 very large, atoms degenerate into 'needles' along the $\underset{\sim}{B}$ field. The generalization of Emden's eqn (1.1) proposed here is only valid for $B \ll Z^3$, but with B still large, having as a consequence a spherically symmetric self-consistent field around the atomic nucleus in the high Z limit.

3 Proposed generalization of Emden's equation

Three of the four equations embraced by the generalized Emden equation

$$\phi'' = \frac{\left\{\phi\left(1+\frac{\gamma\phi}{x}\right)\right\}^{n/2}}{x^{m/2}} \ , \tag{3.1}$$

which is the main focus of the present investigation, have now been stated, namely eqn (1.3) known to Milne [1], eqn (2.8) known to Kadomtsev [12] and eqn (2.6) derived by Hill et al. [10]. These equations correspond respectively to the pairs $[n, m] = [3, 1]$ and $[1, -1]$, with also $\gamma = 0$ for eqns (1.3) and (2.8) and $[n, m] = [1, -1]$ with $\gamma \neq 0$ for eqn (2.6). These pairs, in fact, are already reproduced by the less general case when $m = n - 2$ in eqn (3.1).

The fourth equation embraced by the proposed eqn (3.1), namely the relativistic generalization of the so-called dimensionless Thomas-Fermi eqn (1.3) is discussed briefly in the Appendix. Again the choice $m = n - 2$ in eqn (3.1) is sufficient to include this fourth eqn (A2).

3.1 Some elementary solutions of eqn (3.1)

It is not our aim here to attempt any detailed discussion of solutions of eqn (3.1) satisfying specific physical boundary conditions (such as, e.g. eqns (1.4) and (1.5) for the differential eqn (1.3)). However, it is worthy of note that, for $\gamma = 0$, eqn (3.1) is solved by

$$\phi(x) = Ax^{\beta} \tag{3.2}$$

where substitution in eqn (3.1) with $\gamma = 0$ readily yields

$$\beta = [4 - m]/[2 - n] \tag{3.3}$$

while

$$A = [\beta(\beta - 1)]^{2/n-2} \tag{3.4}$$

For the pair $[n, m] = [3, 1]$ plus $\gamma = 0$, $\beta = -3$ while $A = (12)^2 = 144$, and one recovers the Sommerfeld solution of eqn (1.3) already referred to.

For $\gamma \neq 0$, this solution generalizes to

$$\phi(\gamma, x) = \frac{144}{x^3}\ f\left(\frac{\gamma}{x^4}\right) \tag{3.5}$$

as discussed by Senatore and March [13] but we shall not go into details here (see, however, the Appendix).

Suffice it to say, before summarizing, that numerical solutions are available for pairs $[n, m] = [3, 1]$ and $[1, -1]$ for $\gamma = 0$ satisfying physical boundary conditions, while for some specific values of γ there are also tabulated results for the same pairs of $[n, m]$.

4 Summary and future directions

The main proposal of the present study is summarized in eqn (3.1), which we term the generalized Emden equation. It has been shown to embrace four equations for the screening function of the nuclear potential energy $-Ze^2/r$, namely eqns (1.3) and (2.8) which are non-relativistic and correspond to $\gamma = 0$, and eqns (2.6) and (A2) which are consistent with the Special Theory of Relativity.

It may, we feel, be of interest in the future to seek more general analytical solutions than we have exposed in section 3.1. Returning to the original Emden eqn (1.1), with n now having the different meaning of the polytrope index, Saslaw [3] notes in his book that closed form solutions of Emden's original eqn (1.1) are known for $n = 0, 1$ and 5.

Examination of eqn (3.1) further with $n/2$ now having these values may be fruitful for $\gamma \neq 0$. Also, the possible appearance of irrational indices for other than the Coulson-March solution (1.6) may be worthy of future study.

But what has been achieved here, following the lead of Milne [1], is to pull together via the proposed eqn (3.1), two fields so apparently diverse as the structure of a gaseous star and the electron theory of heavy positive atomic ions, with and without applied magnetic fields.

Acknowledgments

The writer wishes to acknowledge that this investigation was brought to fruition during a visit to the Abdus Salam International Centre for Theoretical Physics, Trieste, Italy, during the year 2000. Special thanks are due to Professor Yu Lu for the very stimulating environment in which to carry out this work, and for generous hospitality. Professor A. Holas is thanked for innumerable valuable discussions in the general area of this study. The work on atomic ions in intense magnetic fields is part of a wider program benefitting from contractual support from the Office of Naval Research. Special thanks are due to Dr. P. Schmidt of that Office for much motivation and his continuing interest.

APPENDIX

Sketch of relativistic generalization of dimensionless Thomas-Fermi eqn (1.3) describing heavy positive atomic ions with $\underset{\sim}{B} = 0$

As in section 3 on the intense magnetic field limit, the starting point is the equation for the relativistic chemical potential μ_α, but now in the zero field limit $B = 0$.

Then, omitting the analogue of eqn (2.1) for μ_α itself, we are led to the equation replacing eqn (2.2) as

$$\frac{(\mu_\alpha - V)^2}{2m_0c^2} + (\mu_\alpha - V(r)) = \frac{1}{2m_0} \cdot \left(\frac{3h^3}{8\pi}\right)^{2/3} \rho^{2/3} \tag{A1}$$

which immediately reduces to the Thomas-Fermi density-potential relation $\rho \propto (\mu_0 - V)^{3/2}$ as $\alpha \to 0$ or equivalently $c \to \infty$.

Making once more the substitution (2.3) but with the length scale $r = bx$ as in the $B = 0$ non-relativistic limit in eqn (1.2), one is led to the equation

$$\phi'' = \frac{\left\{\phi\left(1 + \gamma\frac{\phi}{x}\right)\right\}^{3/2}}{x^{1/2}} : \gamma = \left(\frac{4}{3\pi}\right)^{2/3} \alpha^2 Z^4 \ . \tag{A2}$$

Eqn (A2), which was already known to Vallarta and Rosen [14], completes the four equations unified by the generalized Emden eqn (3.1).

It may be noted here, returning to the Senatore-March solution $144/x^3 f(\gamma/x^4)$, that these workers [13] found that $f(s)$ has a simple pole at a critical value, say s_c, which is $\sim 10^{-2}$. The analogue of the Coulson-March solution (1.6) is readily established then to be of the form

$$\phi(\gamma, x) = \frac{144}{x^3}\ f(\gamma/x^4)\left\{1 - \frac{F_1}{x^c} + \ldots\right\} \ . \tag{A3}$$

The non-zero value of γ will eventually introduce integral inverse powers of x into eqn (A3), but this will only occur at order $1/x^4$.

Also noteworthy is the fact that, as is customary in relativistic atomic theory, it is important to solve eqn (A2) numerically with the inclusion of a finite sized nucleus. In particular, this escapes from a difficulty of the original Vallarta-Rosen scheme [14] that the electron density $\rho(r)$ could not be normalized due to its strong divergence at a (point) atomic nucleus.

References

[1] Milne E A 1927 Proc. Camb. Phil. Soc. **23** 794

[2] Emden R 1907 Gaskugeln (Leipzig and Berlin: B.G. Teubner)

[3] Saslaw W C 1985 Gravitational physics of stellar and galactic systems (Cambridge: University Press)

[4] March N H 1957 Advances in Physics **6** 1

[5] Thomas L H 1926 Proc. Camb. Phil. Soc. **23** 542

[6] Fermi E 1928 Zeits für Physik **48** 73

[7] See also March N H 1975 Self-consistent fields in atoms (Oxford: Pergamon)

[8] Sommerfeld A 1932 Zeits für Physik **78** 283

[9] Coulson C A and March N H 1950 Proc. Phys. Soc. **A63** 367

[10] Hill S H, Grout P J and March N H 1985 J. Phys. B At. Mol. Phys. **18** 4665

[11] Lieb E H, Solovej J P and Yngvason J 1992 Phys. Rev. Lett. **69** 749

[12] Kadomtsev B B 1970 Sov. Phys. - JETP **31** 945

[13] Senatore G and March N H 1985 Phys. Rev. **A32** 3277

[14] Vallarta M S and Rosen N 1932 Phys. Rev. **41** 708