ASYMPTOTIC SOLUTION OF THE THOMAS-FERMI EQUATION

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Abstract

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MATHEMATICS

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As is known ([1]), the solution of the Thomas–Fermi equation

$$\varphi'' = \frac{\varphi^{1.5}}{x^{0.5}}, \tag{1}$$

which determines the statistical distribution of electrons in an atom, must satisfy the boundary conditions:

$$\varphi(0) = 1; \tag{2a}$$

$$\varphi(x = \infty) = 0; \tag{2b}$$

$$\varphi'(x = \infty) = 0. \tag{2c}$$

The boundary conditions (2b) and (2c) are satisfied by the particular solution

$$\varphi_0 = \frac{144}{x^3}. \tag{3}$$

Taking, in order to simplify further calculations,

$$\varphi = \frac{144}{x^3 z^4}, \tag{4}$$

and differentiating (4) and substituting into (1), we obtain

$$z\,(x^2 z'' - 3z) - xz'(5xz' + 6z) + 3 = 0. \tag{5}$$

In order that some solution of equation (5), upon substitution into (4), lead to a function φ satisfying the boundary conditions (2b) and (2c), it is sufficient that this solution tend to unity as $x \to \infty$.

Suppose that equation (4) has a solution representable in the form of a power series

$$z = 1 + a_1 x^{\alpha} + a_2 x^{2\alpha} + a_3 x^{3\alpha} + \ldots + a_{nx}^{n\alpha} + \ldots \tag{6}$$

For the coefficients a_n $(n = 1, 2, \ldots)$ we obtain the recurrence relations

$$\begin{aligned} 0 = a_n[n^2\alpha^2 - 7n\alpha - 6] + a_1 a_{n-1}[(n^2 - 12n + 12)\alpha^2 - 7n\alpha - 6] + \ldots \\ \ldots + a_{ka_{n-k}}[(n^2 - 12nk + 12k^2)\alpha^2 - 7n\alpha - 6] + \ldots \\ \ldots + a_{(n-1)/2} a_{(n+1)/2}[(3 - 2n^2)\alpha^2 - 7n\alpha - 6] \end{aligned} \tag{7a}$$

in the case where n is odd, and

$$a_n[n^2\alpha^2 - 7n\alpha - 6] + a_1 a_{n-1}[(n^2 - 12n + 12)\alpha^2 - 7n\alpha - 6] + \cdots$$

$$\cdots + a_{ka_{n-k}}[(n^2 - 12nk + 12k^2)\alpha^2 - 7n\alpha - 6] + \cdots$$

$$\cdots + a_{n/2-1} a_{n/2+1}[(12 - 2n^2)\alpha^2 - 7n\alpha - 6] + a_{n/2}^2(n^2\alpha^2 + 3.5n\alpha + 3) = 0 \tag{7b}$$

in the case where n is even. The coefficient a_1 remains arbitrary. The exponent α is determined from the equation

$$\alpha^2 - 7\alpha - 6 = 0,$$

whence $\alpha_1 = -0.772$ and $\alpha_2 = 7.772$.

It is obvious that the solution (6), as $x \to \infty$, approaches unity if $\alpha = -0.772$. In this case, after determining the coefficients of the series (6) from (7a) and (7b), we have

$$z = 1 + a_1 x^{-0.772} - 0.00279 a_1^2 x^{-1.544} +$$

$$+0.0_{32279} a_1^3 x^{-2.316} - 0.0_{42814} a_1^4 x^{-3.088} + \cdots, \tag{8}$$

whence, returning to the variable φ, we have

$$\varphi = \frac{144}{x^3 \left(1 + a_1 x^{-0.772} - 0.00279 a_1^2 x^{-1.544} + \cdots\right)^4}. \tag{9}$$

We do not present an investigation of the convergence of the series (8). For practical use of the solution (9) in the statistical theory of atoms, it is possible to restrict oneself to 4 terms of the expansion of the series (8).

If one takes the numerical value of φ at $x = 1$, in accordance with the most reliable data, to be 0.425, then from (9) we find $a_1 = 3.316$, and finally:

$$\varphi = \frac{144}{x^3 \left(1 + 3.316x^{-0.772} - 0.03067x^{-1.544} + 0.00831x^{-2.316} - 0.00340x^{-3.088}\right)^4}. \tag{10}$$

Comparison of the values of φ calculated from (10) with the data of Bush and Caldwell ([2]), obtained on an integrating machine, showed that: 1) for $0.375 < x < 0.75$, formula (10) gives values differing from the data of Bush and Caldwell by no more than 0.5%; 2) for $x \geq 0.75$, formula (10) gives values coinciding with the data of Bush and Caldwell to three significant figures. For values $x < 0.375$, solution (10) is not applicable. However, for very small values of x, the Thomas-Fermi equation itself is not applicable for describing the structure of atoms ([1,3]). Therefore solution (10) may be useful in the statistical theory of atoms within the limits of applicability of the Thomas-Fermi atomic models.

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CITED LITERATURE

1. G. Gombash, *Statistical Theory of the Atom and Its Applications*, IL, 1951. 2. V. Bush, S. H. Caldwell, Phys. Rev., (2) **38**, 1898 (1931). 3. L. Landau, E. Lifshitz, *Quantum Mechanics*, part 1, 1948.

Note: Figure translations are in progress. See original paper for figures.