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Approximate Solution of the Thomas–Fermi Equation for Free Positive Ions

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Abstract: The approximate solution of the nonlinear Thomas–Fermi (TF) equation for ions is found by the Fermi method. The solution is based on the new asymptotic representation of the TF ion size valid for any ionization degree. The two universal functions and their derivatives, introduced by Fermi, are calculated by recent effective algorithms for the Emden–Fowler type equations with the accuracy sufficient for majority of applications. The comparison of our results with those obtained previously shows high accuracy and validity for arbitrary values of ionization degree. This study could potentially be of interest for the statistical TF method applications in physics and chemistry.

Keywords: Thomas–Fermi equation; free positive ion; asymptotic representation; approximating functions

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1. Introduction

The Thomas–Fermi (TF) statistical approach [1–28] is widely used in studies of many-electron systems (atoms, ions, molecules, metals, crystals). By virtue of its importance for physics and chemistry, the TF equation (TFE) was solved by different methods – analytically, semi-analytically, and numerically [1–28]. The results of these numerous and diverse studies show that maximum accuracy is achieved by the analytical-numerical methods [13–17,19–28].

In the TF statistical model [8], the electrostatic potential V within the ion with N bound electrons and nuclear charge Z is defined by the expression

$$V = \frac{Ze}{r}\phi + V_0,$$

where $V_0 = (Z - N)e/r_0$ is the potential at the TF ion boundary r_0. The $\phi(x)$ is the TF function that satisfies the TF equation, where $x = r/r_{TF}$ is measured in TF unit $r_{TF} = \frac{1}{4}(\frac{9\pi^2}{2Z})^{1/3}a_0$, a_0 is the Bohr radius. This nonlinear ordinary differential equation (ODE), which is the foundation of TF method, has the following dimensionless form:

$$x^{1/2}\phi'' = \phi^{3/2}, \tag{1}$$

together with boundary conditions $\phi(0) = 1$ and $\phi(x_0) = 0$. Here, $x_0 = r_0/r_{TF}$ – is the dimensionless ion size (boundary radius) in the TF model, which has to satisfy the condition

$$-x_0\phi'(x_0) = q. \tag{2}$$

The ionization degree q is determined by the number of bound electrons N and nuclear charge Z: $q = (Z - N)/Z$. It could be formally shown that if $N = Z$, and hence $q = 0$ (i.e., for neutral atom), the dimensionless boundary radius x_0 stems to infinity. In this case, the Equation (1) will determine the TF function for the neutral atom. Conventionally, this solution is designated by the function ϕ_0, and it is evidently universal for all Z.

For the free positive ions, the TF Equation (1) solution $\phi(x)$ depends only on the ionization degree q. According to Fermi [4], the approximate solution of (1) could be represented as a sum of two functions

$$\phi(x) = \phi_0(x) + \delta(x), \tag{3}$$

where $\delta(x)$ is assumed small in comparison with the function $\phi_0(x)$. It is evident, that $\delta(0) = 0$. Expanding the right hand side part of (1) in series up to the first order over δ/ϕ_0, with account of (3), one can get the linear ODE for δ:

$$\delta'' = \frac{3}{2}\left(\frac{\phi_0}{x}\right)^{1/2}\delta. \tag{4}$$

Next, it is assumed [4] that

$$\delta(x) = k(q) \cdot \eta_0(x), \tag{5}$$

where $k(q)$ – is the coefficient depending on the ionization degree q, while $\eta_0(x)$ – is the universal function independent from q. Then it follows from (4)

$$\eta_0'' = \frac{3}{2}\left(\frac{\phi_0}{x}\right)^{1/2}\eta_0, \tag{6}$$

with the initial conditions $\eta_0(0) = 0$ and $\eta_0'(0) = 1$. The solution of Equation (6), satisfying the fitting boundary conditions, could be put in the form [4]

$$\eta_0 = \left(\phi_0 + \frac{x\phi_0'}{3}\right)\int_0^x \left(\phi_0 + \frac{t\phi_0'}{3}\right)^{-2} \mathrm{d}t. \tag{7}$$

The values of $\eta_0(x)$ and $\eta_0'(x)$ could be determined as from (7), as by the direct numerical integration of (6) [4]. The latter way was realized in [5,6,8–12], and the results were tabulated. The interpolation formulas for the coefficient $k(q) < 0$ were proposed as well. So, in [6] $k = -0.083q^3$, and in [12] $k = -0.0542q^{2.86}$. However, such interpolation expressions as shown in the present work give satisfactory results only in the range of values $q \leq 0.3$.

A relatively simple analytical approximate solution of Equation (4), applicable for the determination of $\phi(x)$ in the interval from 0 to x_0, was obtained by Sommerfeld in [7]:

$$\phi = \frac{1}{(1+z)^{\lambda_1/2}}\left[1 - \left(\frac{1+z}{1+z_0}\right)^{\lambda_1/\lambda_2}\right], \tag{8}$$

here $z = \left(\frac{x}{\sqrt[3]{144}}\right)^{\lambda_2}$, $\lambda_1 \approx 7.772$ and $\lambda_2 \approx 0.772$. The equation for determination of z_0 and the boundary ion radius x_0 follows from (2) and (8):

$$\frac{z_0}{(1+z_0)^{\lambda_1/2+1}} = \frac{q}{\lambda_1}. \tag{9}$$

The expression in front of the square brackets in (8) is the Sommerfeld approximate solution of TFE for the neutral atom ϕ_0 [7]. The solution (8) of Equation (1) could be significantly improved if the exact numerical values are used for the function ϕ_0 [8]. Then, if to perform the corresponding replacement, Equation (9) for the determination of $z_0(x_0)$ is changed

$$\frac{z_0}{1+z_0}\phi_0(x_0) = \frac{q}{\lambda_1}. \tag{10}$$

However, as was established in the present work, the $x_0(q)$ dependence determination from Equations (9) and (10) is possible only for values of q less than certain $q_{\max}$.

The representation (3) for ϕ is formally invalidated if the correction δ becomes comparable with the value of ϕ_0, i.e., for values of x close to x_0. In order to avoid this and improve the approximate solution of Equation (1) according to the Fermi method, Gombas [8] proposed to define the coefficient $k(q)$ from the equality $\phi(x_0) = \phi_0(x_0) + k\eta_0(x_0) = 0$, that is

$$k = -\frac{\phi_0(x_0)}{\eta_0(x_0)}, \tag{11}$$

using the exact values of boundary radius x_0. However, the exact values of x_0 are not known beforehand and should be determined during the procedure of the solution of Equation (1) taking into account (2). This complexity could be overcome using the asymptotic representation for $x_0(q)$.

The aim of the present paper is an improvement of the Fermi method for solution of Equation (1) for the positive ions in order to get results applicable for practically any values of q with adequate accuracy for applications. That is why the functions $\phi_0(x)$, $\eta_0(x)$ and their derivatives were calculated with high accuracy by the recently developed algorithms [27,28] and tabulated (see Appendix A). The coefficients $k(x_0)$ are determined from (11) based on tabulated values of $\phi_0(x)$ and $\eta_0(x)$, presented in the Appendix A (see Section 2). The asymptotic representation is obtained for the dependence $x_0(q)$ and hence for $k(q)$, applicable for the wide range of the q variation and convenient in practical use (see Section 3). The comparison of $k(q)$ and $x_0(q)$ dependencies with those obtained from the direct numerical solution of TFE and other known data is performed (see Section 3). The accuracy estimations of the derived approximate solution are also presented in the Section 3. The obtained results are summarized in Section 4.

2. Calculations of $k(q)$ Coefficients

The coefficient k (see expression (5)) is the necessary element of the approximate solution of Equation (1) with the help of the representation (3). As we pointed out in the introduction, this coefficient could be determined from the equality $k = -\phi_0(x_0)/\eta_0(x_0)$. In addition, x_0 and k depend on the ionization degree q. The exact value of boundary radius x_0 for an arbitrary ion is not known beforehand, as it determined from the additional condition (2) during the solution of Equation (1). There are two ways to avoid this difficulty. The first version is to find the numerical solution of Equation (1) together with x_0 for some values of the ionization degree, and after k, and next with the help of interpolation to find those quantities for any q. The second one is to use for $x_0(q)$ the asymptotic representation. Both versions are considered below.

Following [10], Equation (1) could be represented via the equivalent system of two ODEs of the first order:

$$\begin{cases} \dfrac{\mathrm{d}p}{\mathrm{d}t} = t \cdot g, \\ \dfrac{\mathrm{d}g}{\mathrm{d}t} = 4p^{3/2}. \end{cases} \tag{12}$$

In (12) $t = \sqrt{x}$, $p(t) = \phi(x)$, $g(t) = 2\phi'(x)$; the initial conditions are: $p(0) = 1$, $g(0) = 2\phi'(0)$. The numerical solutions of the system (12) for different $\phi'(0)$ were found by the Runge–Kutta method of the eighth order [29]. The values of x_0 (condition (2)) and k (the equality (11) and data from Tables A1 and A2) were determined correspondingly and presented in the Table 1 (compare with [12,16]).

The dependence of k coefficient on the ionization degree q is shown in Figure 1. The solid line corresponds to k values shown in Table 1. The dotted curve corresponds to results obtained in [12] for the k values in the course of numerical solution of Equation (1). The dashed curve and the dash-dotted one are related to the two interpolation formulas, $k = -0.083q^3$ [6] and $k = -0.0542q^{2.86}$ [12], respectively. It is seen clearly in the figure that these interpolation formulas suit well only for q less than 0.3. The k values obtained in this work and shown in the Table 1 correspond well to data from [12]. However, it is worth noting that the data of Table 1 encircle the ionization degree values $0.01 \leq q \leq 0.99$, in contrast to [12], where the k values are calculated only for $q \leq 0.65$.

Table 1. The boundary ion radius x_0 and k coefficient (Equation (11)), corresponding to the different values of the ionization degree q, are calculated using the numerical solution of the ODE system (12).

q	x_0	$\log_{10}(\|k\|)$	q	x_0	$\log_{10}(\|k\|)$	q	x_0	$\log_{10}(\|k\|)$
0.01	34.2658	−6.999	0.34	4.5050	−2.383	0.67	1.8529	−1.131
0.02	25.1693	−6.160	0.35	4.3823	−2.336	0.68	1.7975	−1.096
0.03	20.7772	−5.660	0.36	4.2642	−2.291	0.69	1.7429	−1.061
0.04	18.0472	−5.303	0.37	4.1502	−2.247	0.70	1.6892	−1.026
0.05	16.1026	−5.021	0.38	4.0397	−2.203	0.71	1.6361	−0.991
0.06	14.6268	−4.789	0.39	3.9335	−2.161	0.72	1.5833	−0.955
0.07	13.4520	−4.591	0.40	3.8302	−2.119	0.73	1.5314	−0.919
0.08	12.4863	−4.418	0.41	3.7307	−2.077	0.74	1.4799	−0.883
0.09	11.6718	−4.264	0.42	3.6340	−2.036	0.75	1.4287	−0.847
0.10	10.9720	−4.125	0.43	3.5400	−1.996	0.76	1.3783	−0.810
0.11	10.3613	−3.998	0.44	3.4488	−1.957	0.77	1.3280	−0.773
0.12	9.8220	−3.882	0.45	3.3606	−1.918	0.78	1.2780	−0.735
0.13	9.3410	−3.774	0.46	3.2743	−1.879	0.79	1.2286	−0.696
0.14	8.9072	−3.673	0.47	3.1905	−1.841	0.80	1.1792	−0.657
0.15	8.5136	−3.579	0.48	3.1089	−1.803	0.81	1.1300	−0.617
0.16	8.1539	−3.490	0.49	3.0293	−1.766	0.82	1.0810	−0.576
0.17	7.8243	−3.405	0.50	2.9519	−1.729	0.83	1.0318	−0.534
0.18	7.5191	−3.325	0.51	2.8761	−1.692	0.84	0.9833	−0.491
0.19	7.2366	−3.249	0.52	2.8019	−1.656	0.85	0.9343	−0.447
0.20	6.9733	−3.176	0.53	2.7298	−1.620	0.86	0.8851	−0.401
0.21	6.7273	−3.107	0.54	2.6589	−1.584	0.87	0.8359	−0.353
0.22	6.4964	−3.039	0.55	2.5895	−1.548	0.88	0.7864	−0.304
0.23	6.2795	−2.975	0.56	2.5217	−1.513	0.89	0.7363	−0.252
0.24	6.0747	−2.913	0.57	2.4555	−1.478	0.90	0.6857	−0.197
0.25	5.8811	−2.852	0.58	2.3901	−1.443	0.91	0.6344	−0.138
0.26	5.6978	−2.794	0.59	2.3262	−1.408	0.92	0.5822	−0.076
0.27	5.5234	−2.738	0.60	2.2635	−1.373	0.93	0.5285	−0.007
0.28	5.3578	−2.683	0.61	2.2020	−1.338	0.94	0.4735	0.068
0.29	5.1998	−2.630	0.62	2.1415	−1.304	0.95	0.4163	0.152
0.30	5.0486	−2.578	0.63	2.0820	−1.269	0.96	0.3561	0.251
0.31	4.9040	−2.527	0.64	2.0232	−1.235	0.97	0.2918	0.371
0.32	4.7655	−2.478	0.65	1.9656	−1.200	0.98	0.2212	0.528
0.33	4.6328	−2.430	0.66	1.9088	−1.165	0.99	0.1383	0.778

Now consider the determination of the $x_0(q)$ asymptotic representation, based on the consideration of the TFE (1) analytical solution for ions in the two limiting cases of low and high ionization degree q.

The construction of a solution of Equation (1) for ions with the low ionization degree ($q \ll 1$) is based on the expansion in powers of small parameter [17,19]. Skipping the details of calculations it is possible to show that, in the present case, the analytical dependence of $x_0(q)$ could be put in the form (see [17,19]):

$$x_0 = \Lambda_0^{2/3} q^{-1/3} \left(1 + \sum_{k=1}^{\infty} d_k q^{k\lambda_2/3} \right), \tag{13}$$

where $\Lambda_0 \approx 32.7294$, $\lambda_2 \approx 0.772$. The first two coefficients of expansion d_k in (13) are $d_1 = -0.91670$ and $d_2 = 0.02608$.

The expansion of solution of Equation (1) in the functional series for ions with the high ionization degree ($q \to 1$) [14,15] over powers of ratio $N/Z = 1 - q \ll 1$ is also known. This approach allows us to obtain the expansion for the boundary radius x_0 in the form:

$$x_0 = \left(\frac{16}{\pi}\right)^{2/3}\left(\frac{N}{Z}\right)^{2/3}\sum_{m=0}^{\infty} x_{0m}\left(\frac{N}{Z}\right)^{m}, \tag{14}$$

where x_{0m} are the certain coefficients of the expansion (14).

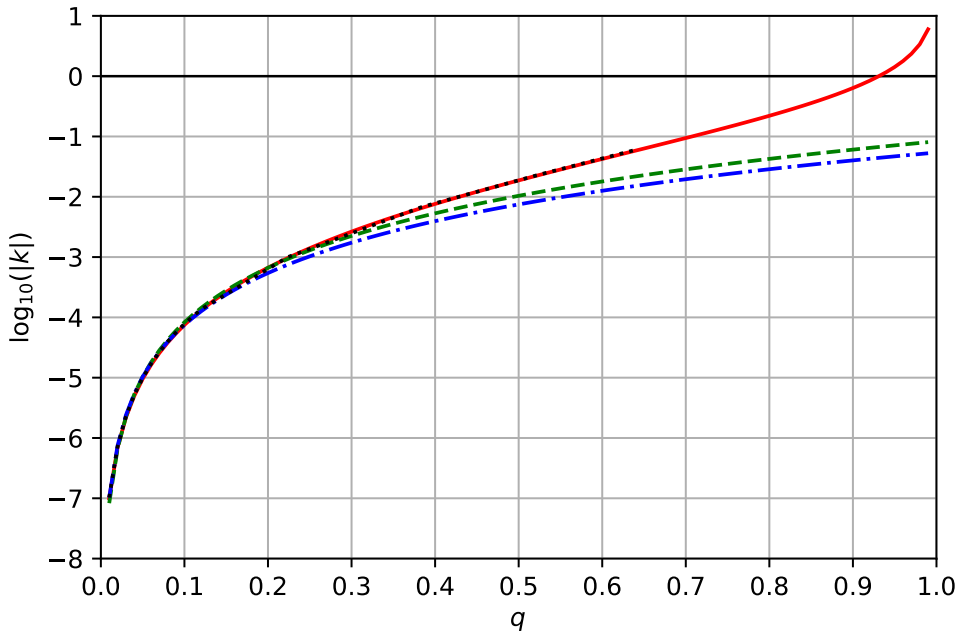

Figure 1. Coefficient k as a function of the ionization degree q. The solid line corresponds to k values shown in the Table 1. The dotted curve corresponds to obtained in [12] k values in the course of numerical solution of Equation (1). The dashed and dash-dotted curves correspond to the two interpolation formulas, $|k| = 0.083q^3$ and $|k| = 0.0542q^{2.86}$ obtained in [6,12], respectively.

The dependence of the boundary radius x_0 on the ionization degree was also studied in the Thomas–Fermi–Dirac model in [20]. By numerical integration of corresponding equations the set of dependencies $x_0(q)$ were obtained for the different values of $Z - N$. It is shown there that for the increasing ionization degree $(Z - N) \to \infty$ $(Z \gg N)$ the set of obtained curves converge to the curve $x_0(q)$, obtained in the TF model without the account of exchange. In so doing, the function $x_0(q)$ has the asymptotics

$$x_0 = \left(\frac{16}{\pi}\frac{1-q}{q}\right)^{2/3}. \tag{15}$$

Joining expressions (13) and (15) it is possible to derive the simple asymptotic representation for $x_0(q)$ suitable for practical calculations

$$\begin{cases} \dfrac{10.232}{q^{1/3}}\left(1 - 0.917q^{0.257}\right), & q \le 0.45; \\ 2.960\left(\dfrac{1-q}{q}\right)^{2/3}, & q > 0.45. \end{cases} \tag{16}$$

The comparison with the data of Table 1 shows that (16) allows us to calculate the $x_0(q)$ values with the root-mean-square error about 0.6% and maximal relative error not exceeding 1.2%.

The dependence of x_0 value on the ionization degree q is presented in the Figure 2. The x_0 values from the Table 1 form the solid line. The dotted curve corresponds to x_0 values, calculated along with the asymptotic representation (16). The dashed and dash-dotted curves are related to solutions of Equations (9) and (10), correspondingly. For

solution of Equation (10) the data of Table A1 for the function $\phi_0(x)$ is used. The analysis of solutions of Equation (9) (the Sommerfeld's solution) and (10) (the solution of Sommerfeld–Fermi) shows that the determination of self-consistent $x_0(q)$ dependence is possible only until the certain limiting value $q_{\max}$. For Equation (9) $q_{\max}$ is around 0.65 and for Equation (10) $q_{\max}$ is about 0.72. However, the Sommerfeld solution corresponds well to the values $x_0(q)$, obtained by the numerical solutions of Equation (1) only for the low ionization degrees $q \leq 0.15$. The modified solution of Sommerfeld–Fermi fits to the numerical $x_0(q)$ values (Table 1) far better, almost up to the corresponding value $q_{\max} \approx 0.72$.

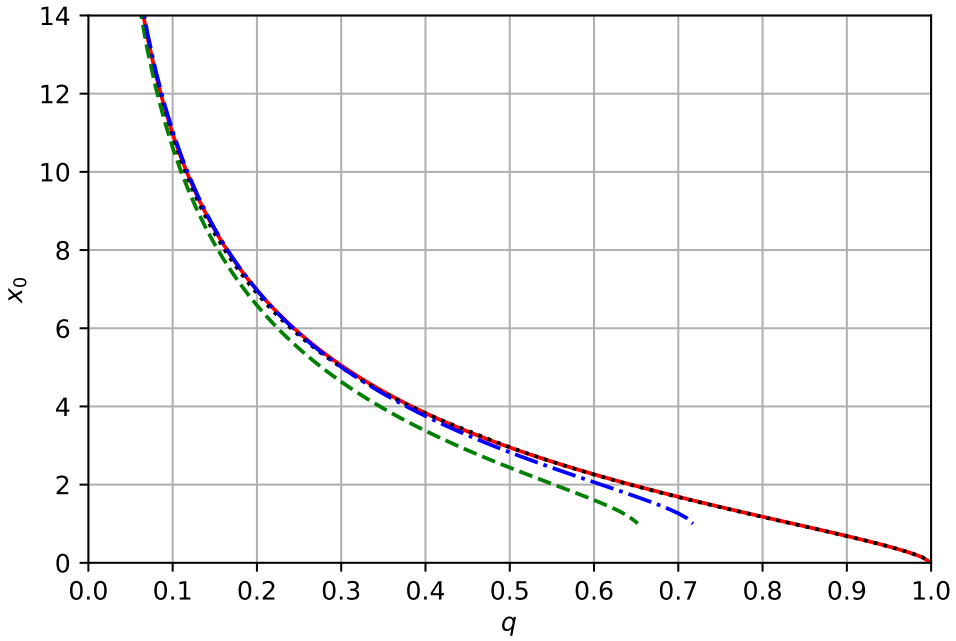

Figure 2. The boundary ion radius x_0 as the function of the ionization degree q. The solid curve corresponds to x_0 values presented in the Table 1. The dotted line is related to the x_0 values calculated using the asymptotic representation (16). The dashed and dash-dotted curves correspond to the solution of Equations (9) and (10), accordingly. In the course of the solution of Equation (10), the data of Table A1 for ϕ_0 were used.

Thus, the results obtained in this section show that application of the asymptotic representation for $x_0(q)$ (16) or the usage of the numerically calculated values of the $k(q)$ coefficients together with the values of functions ϕ_0 and η_0 from Tables A1 and A2 allows us to find approximate solution of Equation (1) for the arbitrary ionization degree q.

3. Approximations of Functions $\phi_0(x)$, $\eta_0(x)$ and Their Derivatives

In cases when the lower accuracy is quite sufficient, it is possible to use the good approximate formulas for functions $\phi_0(x)$ and $\eta_0(x)$ instead of the interpolation of known tabulated data (Tables A1 and A2). For example, the representation of $\phi_0(x)$ in terms of the rational functions from [13] is well known

$$\phi_0(x) = \left(\frac{1 + 1.81061x^{1/2} + 0.60112x}{1 + 1.81061x^{1/2} + 1.39515x + 0.77112x^{3/2} + 0.21465x^2 + 0.04793x^{5/2}} \right)^2 \quad (17)$$

The comparison with the data of Table A1 shows that such approximate formula allows to calculate the values of function $\phi_0(x)$ with the root-mean-square error about 0.2% and the maximal relative error not exceeding 0.5%.

For the function $\eta_0(x)$, we obtained the new approximate formula with the help of the least-square method

$$\eta_0(x) = \exp\left(z + 0.3837z^2 + 0.0892z^3 - 0.0170z^4\right) - 1, \quad z = \ln(1+x) \tag{18}$$

The estimate of accuracy of the Formula (18) for the values of functions $\eta_0(x)$ and $\eta_0'(x)$ along with the data of Table A2 gives the root-mean-square error about 4% and maximal relative error not exceeding 8%. For example, the graphics of functions $\eta_0(x)$ and $\eta_0'(x)$, based on the data of Table A2 are shown in the Figure 3 in solid lines, and using the approximate Formula (18) in dashed lines.

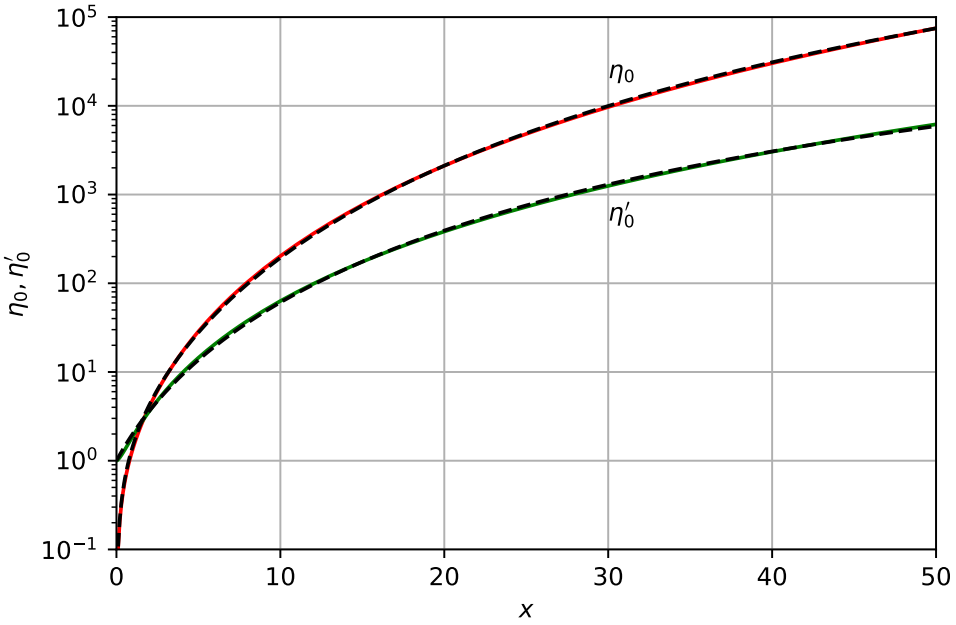

Figure 3. The graphics of functions $\eta_0(x)$ and $\eta_0'(x)$, drawn using the data of Table A2 (**solid lines**) and the approximate Formula (18) (**dashed lines**).

Thus, it is possible to construct the approximate solution of Equation (1) for any value of the ionization degree q (with the accuracy sufficient for the majority of applications). In order to do this, by setting the q value, it is necessary to determine the value of the boundary radius x_0 with the help of the representation (16). After that, the value of coefficient k is determined from the relation (11) and the approximate Formulas (17) and (18). Finally, the solution of Equation (1) for given q is formed from the expressions (5), (3) with the account of (17) and (18).

The graphics of functions $\phi(x)$ and $\phi'(x)$ using the numerical solution of the ODE system (12) (solid lines) and using the approximate solutions (17) and (18) (dotted lines) are shown in the Figure 4 for the different values of the ionization degree: q = 0.2, 0.4, 0.6 and 0.8. The dash-dotted lines are the functions ϕ_0 and ϕ_0' (for a neutral atom), plotted using the data of Table A1. It could be concluded that, in total, this approximate method of the solution construction provides quite good results. The noticeable deviation of the approximate solution from the exact numerical one is seen only for the function $\phi'(x)$ near the ion boundary only for $q > 0.8$. Also, the study demonstrates the consistency of the boundary conditions (2) and (11), although they are functionally different from each other.

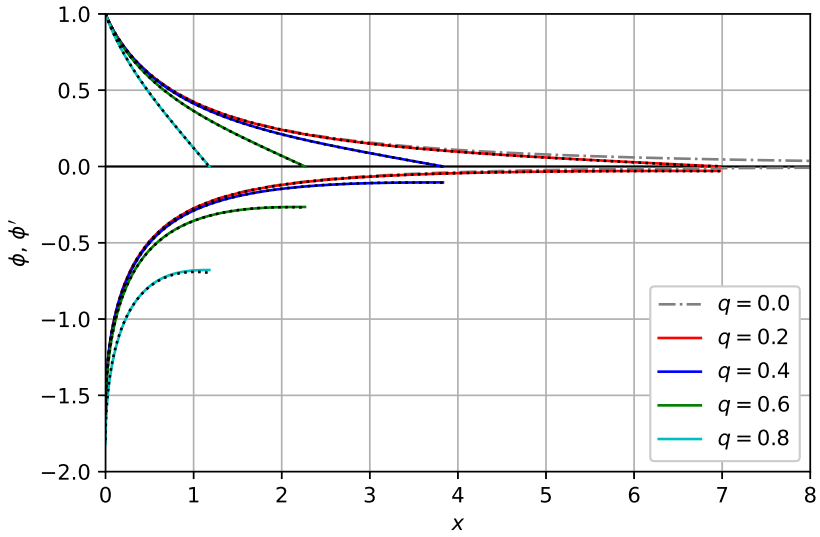

Figure 4. The graphics of functions $\phi_0(x)$ and $\phi_0'(x)$, based on the numerical solution of the ODE system (12) (**solid lines**) and on the base of the approximate formulas (**dotted lines**). The curves for the different values of ionization degree are presented: q = 0.2, 0.4, 0.6 and 0.8. The dash-dotted lines show the curves for functions ϕ_0 and ϕ_0' based on the Table A1 data.

4. Conclusions

The approximate ϕ solution for the free positive ions of the TF equation was found by the E. Fermi method [4] in the assumption of the ϕ representation in the form: $\phi = \phi_0 + k \cdot \eta_0$.

The values of functions ϕ_0 and η_0 are calculated by the new effective analytical-numerical algorithm [27,28] with high accuracy. The obtained values of ϕ_0, η_0 and their derivatives are given in Tables A1 and A2.

The new asymptotic representation of the boundary ion radius $x_0(q)$ is obtained. The values of k coefficient are determined from the numerical solution of TFE for ion using the asymptotic representation for $x_0(q)$. The values $x_0(q)$ and $k(q)$ are presented in Table 1. Note that data of the Table 1 most fully cover the range of the ionization degree values $0.01 \leq q \leq 0.99$, in distinction from other known papers.

The results of the direct $k(q)$ numerical calculations of this work show that the validity of known earlier interpolation formulas for k are limited by values: $q < 0.3$.

Moreover, it follows from the analysis of the other approximate solutions of Equation (1) performed here (Sommerfeld solution (9) and Sommerfeld–Fermi solution (10)) that the determination of the $x_0(q)$ dependencies in these solutions is possible only up to the certain limit value $q_{\max}$. For Equation (9) $q_{\max} \approx 0.65$, and for Equation (10) $q_{\max} \approx 0.72$.

The simple analytical approximation of $\eta_0(x)$ is obtained, which along with the known analytical approximation of $\phi_0(x)$ and the obtained here asymptotics of $x_0(q)$ dependence opens possibility for the approximate solution of the Equation (1) for any value of ionization degree q with an accuracy sufficient for major applications. The estimations of the accuracy of the obtained approximate solution confirm that in total this approach ensures very good results.

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Appendix A. Calculation of Functions $\phi_0(x)$, $\eta_0(x)$ and Their Derivatives

Here we used results [27,28], based on the parametric representation of TFE solution, introduced and applied in the even unpublished paper of E. Majorana, reconstructed along with his notes in [21]. The main peculiarities of this approach are described in [21]. It was recently rigorously mathematically developed and generalized on the Emden–Fowler type of equations in [27,28], where the detailed step by step description of the solution construction is given.

In [27,28] the algorithm of computing the TFE solution and its derivative of the many-electron neutral atom and for the given in advance any accuracy value in arbitrary point of ray is described in detail. We realized this algorithm for computing $\phi_0(x)$ and $\phi_0'(x)$ for the interval $x \in [0, 50]$, but don't repeat its rather lengthy description, referring to original papers [27,28]. We present in Table A1 only the exact values of functions $\phi_0(x)$ and $\phi_0'(x)$ rounded to the tenth decimal sign (compare with [10,24]). It is worth to indicate only that in this algorithm the corresponding subsidiary functions of the parametric representation [27,28] are expanded in the Taylor series that in our case contained 120 terms.

Table A1. Values of functions $\phi_0(x)$ and $\phi_0'(x)$ calculated on the basis of the method from [27,28] and rounded to the tenth decimal sign.

x	$\phi_0(x)$	$-\phi_0'(x)$	x	$\phi_0(x)$	$-\phi_0'(x)$
0.00	1.0000000000	1.5880710226	10.00	0.0243142930	0.0046028819
0.01	0.9854466129	1.3895561166	11.00	0.0202503650	0.0035798152
0.02	0.9719766389	1.3093049632	12.00	0.0170639223	0.0028305364
0.05	0.9351919580	1.1559954352	13.00	0.0145265176	0.0022705246
0.10	0.8816970767	0.9953546461	14.00	0.0124784060	0.0018445014
0.20	0.7930594320	0.7942270092	15.00	0.0108053588	0.0015153231
0.30	0.7206394761	0.6617997801	16.00	0.0094240789	0.0012574353
0.40	0.6595411608	0.5646424441	17.00	0.0082727639	0.0010528868
0.50	0.6069863834	0.4894116126	18.00	0.0073048459	0.0008888311
0.60	0.5611620236	0.4291718717	19.00	0.0064847464	0.0007559214
0.70	0.5207914565	0.3797947453	20.00	0.0057849412	0.0006472543
0.80	0.4849309880	0.3386071561	21.00	0.0051838934	0.0005576616
0.90	0.4528587154	0.3037757561	22.00	0.0046645758	0.0004832257
1.00	0.4240080521	0.2739890516	23.00	0.0042133981	0.0004209437
1.10	0.3979253017	0.2482781190	24.00	0.0038194181	0.0003684892
1.20	0.3742412296	0.2259085936	25.00	0.0034737544	0.0003240430
1.30	0.3526512782	0.2063121826	26.00	0.0031691444	0.0002861695
1.40	0.3329013700	0.1890414262	27.00	0.0028996077	0.0002537267
1.50	0.3147774637	0.1737387990	28.00	0.0026601879	0.0002257990
1.60	0.2980977070	0.1601150078	29.00	0.0024467526	0.0002016471
1.70	0.2827064352	0.1479333856	30.00	0.0022558366	0.0001806700
1.80	0.2684695100	0.1369984380	31.00	0.0020845191	0.0001623762
1.90	0.2552706498	0.1271472890	32.00	0.0019303255	0.0001463611
2.00	0.2430085072	0.1182431916	33.00	0.0017911496	0.0001322900
2.20	0.2209499788	0.1028309760	34.00	0.0016651908	0.0001198846
2.40	0.2017027012	0.0900262759	35.00	0.0015509032	0.0001089121
2.60	0.1848021494	0.0792857632	36.00	0.0014469544	0.0000991772
2.80	0.1698782637	0.0702003884	37.00	0.0013521916	0.0000905149
3.00	0.1566326732	0.0624571309	38.00	0.0012656139	0.0000827855
3.40	0.1342470024	0.0500771162	39.00	0.0011863493	0.0000758704
3.80	0.1161656951	0.0407527383	40.00	0.0011136356	0.0000696680
4.20	0.1013578688	0.0335900970	41.00	0.0010468047	0.0000640915
4.60	0.0890854399	0.0279948614	42.00	0.0009852690	0.0000590661
5.00	0.0788077793	0.0235600750	43.00	0.0009285103	0.0000545274
5.50	0.0681603623	0.0192213484	44.00	0.0008760706	0.0000504195
6.00	0.0594229493	0.0158675495	45.00	0.0008275439	0.0000466941
6.50	0.0521729373	0.0132356072	46.00	0.0007825691	0.0000433088
7.00	0.0460978186	0.0111425318	47.00	0.0007408251	0.0000402270
7.50	0.0409624662	0.0094582646	48.00	0.0007020247	0.0000374164
8.00	0.0365872553	0.0080886030	49.00	0.0006659114	0.0000348487
9.00	0.0295909353	0.0060330747	50.00	0.0006322548	0.0000324989

In our work the functions $\eta_0(x)$, $\eta_0'(x)$ are obtained by the direct numerical integration of the system of two ODE of the first order, equivalent to (6):

$$\begin{cases} \dfrac{du}{dt} = t \cdot v, \\ \dfrac{dv}{dt} = 6\sqrt{\phi_0(t)} \cdot u. \end{cases} \tag{A1}$$

Here $u(t) = \eta_0(x)$, $v(t) = 2\eta_0'(x)$ and $t = \sqrt{x}$. Note that Fermi [4] used namely this Equation (6) for the determination of the functions $\eta_0(x)$, $\eta_0'(x)$. The system (A1) should be supplemented by the initial conditions $u(0) = 0$ and $v(0) = 2$. The integration of system (A1) was performed by the explicit Runge-Kutta method of the eighth order [29]. The calculated in this way functions $\eta_0(x)$ and $\eta_0'(x)$ are presented in Table A2 (compare with [11]).

Table A2. The values of functions $\eta_0(x)$ and $\eta_0'(x)$, obtained in the course of solution of the system of Equations (A1). For the function $\phi_0(x)$ the data from Table A1 is used.

x	$\eta_0(x)$	$\eta_0'(x)$	x	$\eta_0(x)$	$\eta_0'(x)$
0.00	0.0000	1.0000	10.00	202.6583	63.1040
0.01	0.0100	1.0010	11.00	273.6843	79.3834
0.02	0.0200	1.0028	12.00	362.3564	98.4141
0.05	0.0502	1.0110	13.00	471.5289	120.4630
0.10	0.1012	1.0306	14.00	604.3719	145.7945
0.20	0.2069	1.0846	15.00	764.3028	174.6881
0.30	0.3186	1.1528	16.00	955.0359	207.4327
0.40	0.4378	1.2321	17.00	1180.5679	244.3242
0.50	0.5654	1.3210	18.00	1445.1810	285.6650
0.60	0.7023	1.4187	19.00	1753.4709	331.7663
0.70	0.8494	1.5246	20.00	2110.3680	382.9501
0.80	1.0075	1.6384	21.00	2521.1430	439.5482
0.90	1.1773	1.7599	22.00	2991.3916	501.8995
1.00	1.3597	1.8889	23.00	3527.0042	570.3437
1.10	1.5554	2.0255	24.00	4134.2403	645.2326
1.20	1.7651	2.1696	25.00	4819.7341	726.9275
1.30	1.9895	2.3212	26.00	5590.4890	815.7977
1.40	2.2295	2.4805	27.00	6453.8716	912.2193
1.50	2.4859	2.6474	28.00	7417.6127	1016.5747
1.60	2.7593	2.8222	29.00	8489.8225	1129.2531
1.70	3.0506	3.0048	30.00	9679.0108	1250.6516
1.80	3.3605	3.1954	31.00	10,994.1034	1381.1762
1.90	3.6899	3.3942	32.00	12,444.4521	1521.2416
2.00	4.0396	3.6012	33.00	14,039.8362	1671.2709
2.20	4.8032	4.0406	34.00	15,790.4536	1831.6937
2.40	5.6582	4.5149	35.00	17,706.9028	2002.9441
2.60	6.6116	5.0253	36.00	19,800.1671	2185.4578
2.80	7.6708	5.5730	37.00	22,081.7477	2379.6860
3.00	8.8434	6.1594	38.00	24,563.5873	2586.0847
3.40	11.5604	7.4537	39.00	27,258.1046	2805.1179
3.80	14.8292	8.9197	40.00	30,178.1922	3037.2577
4.20	18.7207	10.5690	41.00	33,337.2044	3282.9824
4.60	23.3105	12.4137	42.00	36,748.9585	3542.7757
5.00	28.6793	14.4660	43.00	40,427.7448	3817.1274
5.50	36.6166	17.3427	44.00	44,388.3414	4106.5335
6.00	46.0833	20.5888	45.00	48,646.0302	4411.4968
6.50	57.2708	24.2302	46.00	53,216.6120	4732.5279
7.00	70.3838	28.2939	47.00	58,116.4192	5070.1454
7.50	85.6401	32.8070	48.00	63,362.3244	5424.8761
8.00	103.2702	37.7972	49.00	68,971.7455	5797.2546
9.00	146.6512	49.3222	50.00	74,962.6446	6187.8231

The minimal value of the ionization degree q of the ion with the nuclear charge Z is determined by the value $q = 1/Z$. The consideration of ions with $Z \approx 100$ is of interest from the practical point of view that corresponds to $q = 0.01$ and the value of boundary ion radius $x_0 \approx 34$ (see Table 1). Thus the represented in Tables A1 and A2 values of functions $\phi_0(x)$, $\phi_0'(x)$, $\eta_0(x)$ and $\eta_0'(x)$ for $x \in [0, 50]$, cover in full all x_0, corresponding to $q \geq 0.01$.

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