Approximate solutions to the Thomas-Fermi equation

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A systematic procedure to construct approximants to the solution of the Thomas-Fermi equation for isolated neutral atoms is presented. The method takes into account the power-series expansions of the solution of the Thomas-Fermi equation for small and large values of the coordinate and matches them. The initial slope is accurately calculated and the approximants are shown to represent the solution for all values of the coordinate with reasonable accuracy. The method is presented in a general way so that it can be applied to other problems of physical interest.

I. INTRODUCTION

The Thomas-Fermi (TF) model provides a semiclassical description of atoms having numerous electrons[1,2] and has also proved to be useful in the study of molecules and crystals.[1] Although it was proposed long ago, it is still a popular model and has been recently applied to atoms in external fields[3] and dense plasmas.[4] Moreover, the TF model has motivated the development of several density-functional theories.[5] There is at least one further reason to study the TF equation: because it is a nonlinear differential equation, the methods used to solve it, either numerically or in an approximate analytic way, may be useful in other fields of theoretical physics in which such equations are commonly found.

Besides accurate numerical calculations,[6-8] there have been proposed several analytic approaches to the solution of the TF equation which exhibit many and various forms.[2] Of these, some are merely guesses in order to find expressions that agree with the numerical results as accurately as possible, but only a few of them take into account the analytic properties of the solution of the TF equation, although not in a systematic way.

Nonlinear differential equations can rarely be solved exactly; even numerical solutions are commonly difficult to obtain. Furthermore, in many cases approximate analytic solutions provide a deeper insight into the physical properties of the system.[9(a),9(b)] Perturbation theory is one of the general approaches proposed to this end.[10] However, as the perturbation equations are commonly complicated, one requires a good deal of ingenuity to solve them. The purpose of this paper is to present a general method to obtain systematic approximants to functions that can be expanded as asymptotic power series; the solutions to many nonlinear differential equations can be treated in this way. The TF equation poses an interesting test problem both because it cannot be solved exactly and because many numerical and approximate analytic results are available.

After the TF equation is briefly discussed in Sec. II, the method is developed in Sec. III in a general way. Results and discussion are found in Sec. IV.

II. THE THOMAS-FERMI EQUATION

According to the TF model, the number of electrons per unit volume in an isolated neutral atom is given by

$$\rho(r)=(8\pi/3h^3)(2me)^{3/2}[V(r)-V_0]^{3/2} ,$$

in which r is the distance from the nucleus, $V(r)$ is the electrostatic potential, and V_0 is a reference value of the potential. The electrostatic potential can be expressed in SI units as

$$V-V_0=-Ze\Phi(x)/(4\pi\epsilon_0) ,$$

in which $x=\gamma r$,

$$\gamma(32\pi^2/3)^{2/3}me^2Z^{1/3}/(2\pi\epsilon_0h^2) ,$$

and $\Phi(x)$ is a solution to the dimensionless equation[1,2]

$$\Phi''(x)=x^{-1/2}\Phi(x)^{3/2}, \quad 0\le x<\infty \tag{1}$$

in which $\Phi(0)=1$. The initial slope $\Phi'(0)$ is to be determined so that $\Phi(\infty)=0$. Let Φ_0 be the exact value of the initial slope corresponding to $\Phi(\infty)=0$ and $\Phi'(0)$ its estimated value. If $\Phi'(0)>\Phi_0$, then $\Phi(x)$ has a pole of order 4 on the real axis.[9(a)] Some of these solutions are used to describe the electronic density of crystals when the sphere approximation is made, and of molecules with high symmetry. On the other hand, if $\Phi'(0)<\Phi_0$, the solution $\Phi(x)$ vanishes at a finite value of x that is considered to be the radius of the ion.[11] We consider here only the case of neutral atoms and apply a systematic method to generate approximate solutions to Eq. (1). In order to make this paper self-contained and the discussion of the results clearer, we first consider some known properties of the solution of the TF equation.

Introducting the new variable $t=x^{1/2}$, we rewrite the TF equation:

$$t\frac{d^2\xi}{dt^2}-\frac{d\xi}{dt}=4t^2\xi^{3/2} , \tag{2}$$

in which $\xi(t)=\Phi(t^2)$. The solution to this equation is expanded in a Taylor series around $t=0$,[11]

$$\xi(t)=\sum_{j=0}^{\infty} a_j t^j , \tag{3}$$

in which $a_0=1$, $a_1=0$, $a_3=\frac{4}{3}$, $a_4=0$, $a_5=2a_2/5$, and

$$a_{n+4}=(n+1)^{-1}[(n+3)^2-1]^{-1} \times \left[\tfrac{3}{2} \sum_{j=1}^{n} (j+1)[(n+2-j)^2-1]a_{j+1}a_{n+3-j} - \sum_{j=0}^{n-2} (j+1)[(j+3)^2-1]a_{j+4}a_{n-j} \right] , \quad n=2,3,\ldots . \tag{4}$$

All the coefficients a_j can be calculated easily in terms of the initial slope a_2 according to this recurrence relation.

In order to obtain the asymptotic behavior of Φ for large values of x one finds it convenient to use the variables $s=x^r$, with $r=(7-73^{1/2})/2$, and to write $\Phi(x)=144x^{-3}v(s)$.[1,9(a),12] The function $v(s)$ satisfies the differential equation

$$r^2 s^2 \frac{d^2 v}{ds^2}+6s\frac{dv}{ds}+12v=12v^{3/2} . \tag{5}$$

Therefore, $v(s)$ can be expanded in a Taylor series around $s=0$,[1,9(a),12]

$$v=\sum_{j=0}^{\infty} v_j s^j , \tag{6}$$

in which $v_0=1$, and

$$v_{n+1}=\{n(n+1)[r^2(n+1)+6]\}^{-1}\sum_{j=0}^{n-1}(j+1)v_{j+1}v_{n-j}\{\tfrac{3}{2}[r^2(n-j)(n-j-1)+6(n-j)+12] -r^2 j(j+1)-6(j+1)-12\}, \quad n=1,2,\ldots . \tag{7}$$

It follows directly from the differential equation (5), that $v_j=c_j v_1^j$, v_1 being unknown. The coefficients c_j can be obtained easily and exactly from (7).

Both a_2 and v_1 are global properties of the TF equation and cannot be obtained from a local analysis of the solution like the expansions (3) and (6). These parameters have been accurately calculated by means of an iterative method based on the series (3) and (6).[2,13] For this purpose these series were modified in order to improve their convergence properties and then matched at $x=1$ under the requirement of analytic continuation. Because the original work[11] is practically inaccessible, we have perforce to refer to its discussion in Ref. 2.

By the method of dominant balance,[9(c)] one can easily prove that $v(s)$ has at least one singular point around which it is asymptotic to $(\frac{25}{9})r^4 s_0^4 (s-s_0)^{-4}$. From the most accurate coefficients of series (6) available in the literature[2,13] together with the ratio method and its variants,[14] we have estimated $s_0\cong -0.300\,51$. As the ratio method determines the singular point closest to the origin, it follows that series (6) is convergent for all $x>4.7462$; the value quoted in Ref. 2 is 4.75. This information is not required to apply our procedure but proves useful to explain the convergence properties of the approximants.

By a simple systematic method developed in Sec. III, we obtain increasingly accurate approximants to the solutions of the TF equation. Although this procedure resembles that discussed above,[2,13] there are important differences. First, in the present method only one series and the first term of the other are used to construct the approximants. To succeed in this goal, we require a greatly improved local representation of the solution. Second, our procedure is presented in a general way so that it can be applied to other problems in theoretical physics and chemistry. In fact, previous and future applications are discussed below. We show here how to apply the method to the TF equation, which is a suitable example of nonlinear differential equations for the reasons given in the introduction.

III. METHOD

In what follows we develop a systematic procedure to obtain approximants to a function $f(x)$ that satisfies two asymptotic expansions. For small values of x it is given approximately by

$$f(x)=\sum_{j=0}^{\infty} f_j x^j ; \tag{8}$$

here it is assumed that a sufficiently large number of coefficients f_j can be calculated. For large values of x the function f is known to be asymptotic to

$$f(x)=x^{\alpha}\sum_{j=0}^{\infty} F_j x^{-\beta j} , \tag{9}$$

in which $\beta>0$. Our objective is to match Eq. (8) and the first term in Eq. (9).

The method is based on the properties of the nonlinear mapping

$$x=Ku/(1-u)^{1/\beta} , \tag{10}$$

in which K is an arbitrary real positive number. The new variable u can be expanded in a power series of either x, $u=x/K+x^2/(\beta K^2)+\cdots$, or $x^{-\beta}$, $u=1-K^{\beta}x^{-\beta}+\cdots$. for small or large values of x, respectively. The transformation (10) maps $0\le x<\infty$ onto $0\le u<1$. Because

$$K^{\alpha}(1-u)^{-\alpha/\beta}=(x/u)^{\alpha}$$

is asymptotic to x^{α} as $x\to\infty$, the approximant

$$g(N,u)=K^{\alpha}(1-u)^{-\alpha/\beta}\sum_{j=0}^{N} g_j(K)u^j \tag{11}$$

satisfies power-series expansions similar to those in Eqs. (8) and (9). Therefore, it is supposed to be a good approximation to f provided that the coefficients g_j and the arbitrary parameter K are properly chosen. For instance, if the first N coefficients of the series (8) are known, then the first N coefficients of the approximant are determined according to the formula

$$g_n = K^{-\alpha} \sum_{j=0}^{n} (-1)^{n-j} \binom{(\alpha - j)/\beta}{n-j} K^j f_j \ , \tag{12}$$

in which

$$\binom{b}{j} = b(b-1)\cdots(b-j+1)/j! \ .$$

The purpose of the adjustable parameter K is either to improve the convergence of the sequence of approximants or to lead to simpler expressions. One can use for convergence several criteria which apply to different cases.[15] We choose here a procedure that is useful when F_0 is known and when the coefficients f_j depend on an unknown parameter a which has to be calculated in order to obtain the desired approximation to f.

When $x \to \infty$,

$$x^{-\alpha} g(N,u) \to (g_0 + g_1 + \cdots + g_N) \ ,$$

and $x^{-\alpha} f(x) \to F_0$. Therefore, for g to be a good approximation to f, at least $(g_0 + g_1 + \cdots + g_N) = F_0$. As K is arbitrary, we can set its value so that

$$\sum_{j=0}^{M} g_j = F_0, \quad M < N \tag{13}$$

in which case

$$\sum_{j=M+1}^{N} g_j = 0 \ . \tag{14}$$

If physically acceptable solutions to Eqs. (13) and (14) exist, then both K and a can be determined from them. The roots of Eq. (14) form a set of sequences, one member for every value of M: $a_2(M,N)$, $M = 0, 1, \ldots$, $N = M+1, M+2, \ldots$. It is desirable that all these sequences converge to the same limit. Even when the sequences are divergent, the method still applies provided that they can be truncated in a proper way, as shown in Sec. IV.

In closing, it is worth mentioning that this method could be easily modified to include series for large values of x of the form

$$f(x) = F(x)(F_0 + F_1 x^{-\beta} + \cdots + F_j x^{-\beta j} + \cdots) \ ,$$

provided that $F(x)$ is analytic at $x = K$.

IV. RESULTS AND CONCLUSIONS

We now apply the method discussed above to the TF equation. We have written programs in REDUCE in order to calculate the coefficients of the series (3) and (6) analytically up to order 35, thus augmenting the set of such coefficients that have been published.[6,8] The series (11) has been treated in the same way. Furthermore, in order to avoid roundoff errors, the roots of Eq. (14) have been computed through a standard Newton-Raphson method written in REDUCE with a precision of 16, 20, or 24 digits.

On comparing the series (3) and (6) with the general results of Sec. III, we conclude that the method there described can be applied to the TF equation when $\alpha = -6$ and $\beta = -2r$. As the first two coefficients of the modified series for small values of x are K^6 and $-3K^6/r$, Eqs. (13) and (14) are clearly simpler when $M = 0$ or 1, because the value of the arbitrary parameter K is immediately found to be $K = 144^{1/6}$ or $K = [144r/(r-3)]^{1/6}$, respectively. When $M > 1$, one has to solve a nonlinear system of two equations with two unknowns, namely, K and a_2. For the sake of simplicity, such cases are not considered here.

When $\beta = -2r$, it is impossible to solve Eq. (10) for u in terms of x; therefore, the approximants are implicit analytic expressions of x. As we do not use the entire series (6) but only its first term, the results may be almost insensitive to the value of β considered in the mapping (10). Therefore, one can choose a value of β that leads to simpler approximants. The choice $\beta = 1$ seems appropriate for two reasons. First, it leads to a parametrized Euler transformation which is known to be useful to improve the convergence properties of power-series expansions.[16] Second, the value $\beta = 1$ is not too far from $-2r \cong 1.54$. In this case the appropriate values of K are $K = 144^{1/6}$ and $(\frac{144}{7})^{1/6}$ for $M = 0$ and $M = 1$, respectively. Hereafter, the four approaches with $\beta = -2r$, $M = 0$, $M = 1$, and $\beta = 1$, $M = 0$, $M = 1$ are designated (A1), (A2), (A3), and (A4), respectively. Because the approximants are chosen to satisfy the Taylor expansion about $t = 0$ and to be asymptotic to $144x^{-3}$ as $x \to \infty$, it is expected that the roots of Eq. (14) converge towards the exact initial slope as $N \to \infty$.

The roots of Eq. (14) for these four cases have been calculated for increasing values of N. We monitor the convergence properties of the sequence of values of a_2 by means of the logarithm of the consecutive differences

$$L_N = \log_{10} |a_2(N) - a_2(N-1)| \ ,$$

which are shown in Fig. 1 for increasing values of N. The cases A1 and A2 tend at first to converge more rapidly than A3 and A4, but A1 shows a strongly divergent behavior after $N = 16$. (Use of varied precision in the calcu-

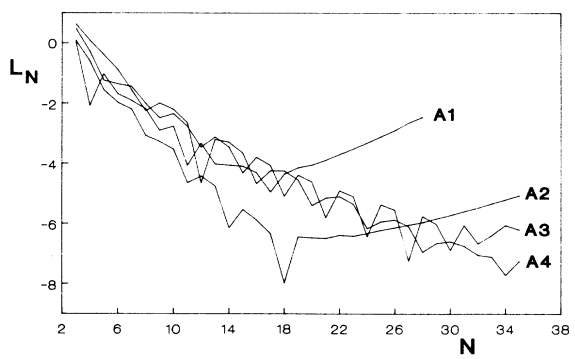

FIG. 1. $L_N = \log_{10}|a_2(N) - a_2(N-1)|$ vs the number N of terms in the approximants for cases A1, A2, A3, and A4.

lations proves that such divergence is not a numerical artifact.) The value of L_N for A2 decreases more rapidly than the others but diverges slowly after $N=18$. In contrast, the behavior of A3 and A4 are remarkably similar; although they converge more slowly than A1 and A2 when $N<16$, their tendencies to converge remain up to $N=30$ and 34, respectively. It is reasonable to assume that the best value of the initial slope that can be obtained from these divergent series is given by $a_2(J-1)$ in which J is the value of N corresponding to the smallest value of L_N. According to this criterion, we obtain the following values of a_2: $-1.588\,070\,322$, $-1.588\,070\,854$, $-1.588\,070\,279$, and $-1.588\,070\,947$ for cases A1, A2, A3, and A4, respectively. The agreement with the nominally accurate result attributed to Rijnierse,[2,13] namely,

$$a_2=-1.588\,071\,022\,600\,00\ ,$$

is remarkable.

Another interesting feature of the method is that the roots of Eq. (14) approach the correct limit even when K is not exactly given by Eq. (13). This fact suggest that the method may still be used even though the first term of the series for large values of x is unknown. This result is not surprising because in summing strongly divergent perturbation series[15(b),15(c)] and in calculating dissociation energies of diatomic molecules from the Dunham coefficients,[17] one obtains the first term of the series for large values of x from the series for small values of x. In these cases the parameter K is determined according to appropriate criteria for convergence.

The approximants with $N=1$, 3, and 5, and $N=3$, 4, and 5 for cases A1 and A2 are shown in Figs. 2 and 3, respectively. Because those approximants with $N=0$ and 1 are independent of a_2, Eq. (14) does not apply to them. When $M=1$ and $N=2$, Eq. (14) reduces to $g_2=0$; for this reason this approximant equals that with $N=1$. Figures 2 and 3 show that the approximants developed here are acceptable approximations to the solution of the TF equation for $0\le x\le 10$. The accuracy decreases for larger values of x but the approximants behave in the same way as the exact solution and vanish as $144x^{-3}$ as $x\to\infty$.

All these results can be markedly improved for small

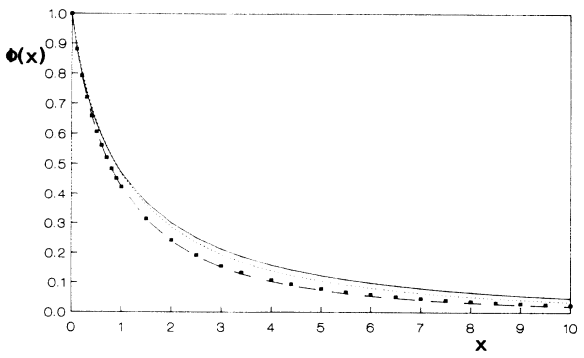

FIG. 2. Approximants to $\Phi(x)$ depending on the number N of terms for $N=1$ (——), $N=3$ (· · · ·), and $N=5$ (— — —) for case A1 [exact values (■)].

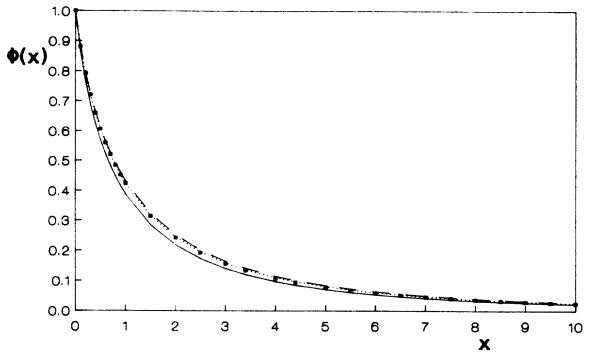

FIG. 3. Approximants to $\Phi(x)$ depending on the number N of terms for $N=3$ (——), $N=4$ (· · · ·), and $N=5$ (— — —) for case A2 [exact values (■)].

values of x by using in all the cases the best value of a_2 that can be obtained from the roots of Eq. (14) as discussed above. However, we have preferred to use in every case the root of Eq. (14) that corresponds to the order of the approximant. The approximants for the cases A3 and A4 lead to results that are similar to those just discussed. However, as noted before, these approximants are preferable if one is interested in simple analytic approximations to the solution of the TF equation. For instance, when $N=2$, we have

$$\Phi(x)=(K+x^{1/2})^{-8}(K^8+8K^7x^{1/2}+144x)\ , \qquad (15)$$

in which $28K^6+a_2K^8=144$. This expression is a reasonably accurate approximation to the solution of the TF equation when the best value of a_2 is used. The electron density for an atom with Z electrons given, for instance, by the approximate screening function (15) is

$$\rho(r)=-(8\pi e^4/3h^3)[mZ/(2\pi\epsilon_0)]^{3/2}[\phi(\gamma r)/r]^{3/2}\ . \qquad (16)$$

One should keep in mind that the approximants discussed here have been obtained by taking into account only the analytic properties of the solution of the TF equation without making reference to numerical results, as is commonly the case in other approximation schemes.[2] For this reason we deem that the procedure developed above may be of general utility in making fruitful use of power-series expansions.

One can in principle apply the method discussed in Sec. III to the series (6) by rewriting Eq. (3) as

$$x^3\xi(t)/144=(s^{3/r}/144)\sum_{j=0}^{\infty}a_j s^{j/(2r)}\ . \qquad (17)$$

This relation shows that $\alpha=3/r$ and $\beta=-1/(2r)$ in this case. However, the roots of Eq. (14) fail to converge as N increases; the reason is probably the singularity at s_0 which, as shown before, is close to the origin. This difficulty could in principle be overcome if one matches at an intermediate point both modified series each containing many terms. However, this procedure, which is expected to lead to more accurate results, would be similar to that of Rijnierse;[2,13] we therefore do not pursue it here.

The parametrized Euler transformation ($\beta=1$) appears to be more promising because the singularity is mapped

into $u_0 = s_0/(s_0+K)$. Therefore, if according to the procedure discussed above,

$$K = 144^{r/3} \cong 0.278\,34\ ,$$

then $|u_0| > 1$; thus the singularity is mapped outside the disk $|u| \leq 1$. As a result, the modified series converges for all values of x provided that no other singularity is mapped into the specified region.

Because of the form of the coefficients v_j discussed in Sec. II, the simplest case is that with $M = 0$; therefore, $K = 144^{r/3}$. As shown in Table I, the roots of Eq. (14) converge slowly and monotonically from below towards the correct value

$$v_1 = -13.270\,973\,848$$

(Refs. 2 and 13). However, the root for $N = 18$ deviates from the sequence and no roots are found for larger values of N. On assuming that the sequence behaves approximately as

$$v_1(N) = v_1(\infty) + c/(N+p)\ ,$$

we have found that $v_1(\infty) = -13.2707$, $c = -2.0281$, and $p = 1.0785$ for $10 \leq N \leq 17$; therefore, $v_1(\infty)$ is an acceptable estimate of the actual value of v_1.

From the point of view of convergence, at least with respect to the singularity at s_0, the most favorable choice appears to be $K = -s_0$ because in this case $|u_0| = \infty$. Although this choice leads exactly to the parametrized Euler transformation that Rijnierse[2,13] used, numerical calculations shows that the sequence for v_1 converges towards an incorrect limit; the reason may be that the first term of series (16) is not taken exactly into account.

In summary, we have developed a systematic method to obtain approximants to functions that can be expanded in power series. Application to the TF equation shows clearly both the advantages of the procedure and some difficulties. The present results and those obtained previously for other examples by means of variants of this technique[15(a),15(b),17] suggest that it may be a useful tool for the study many other physical problems. For instance, the approximants prove to be powerful to fit experimental data when there is a theory for the local behavior of the physical property for small and large values of the variable.[19]

TABLE I. Sequence of values of v_1.

N	$v_1(N)$
2	−13.807 742 840 090 32
3	−13.705 956 144 239 76
4	−13.635 937 825 256 53
5	−13.585 043 690 434 95
6	−13.546 290 300 304 49
7	−13.515 731 429 442 14
8	−13.490 988 474 405 61
9	−13.470 536 411 412 31
10	−13.453 347 515 297 08
11	−13.438 701 347 310 91
12	−13.426 076 599 913 60
13	−13.415 086 080 770 45
14	−13.405 435 842 692 71
15	−13.396 898 524 831 58
16	−13.389 295 404 837 21
17	−13.382 492 145 467 69
18	−10.021 795 868 349 70

As a rigorous and general mathematical proof of the convergence properties of the approximants may prove difficult, further applications will be necessary to establish the general validity of the method. One possible application is the calculation of eigenvalues from the Riccati equation satisfied by the logarithmic derivative of the wave function.[19]

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