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The Thomas–Fermi Problem and Solutions of the Emden–Fowler Equation

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Abstract—A two-point boundary value problem is considered for the Emden–Fowler equation, which is a singular nonlinear ordinary differential equation of the second order. Assuming that the exponent in the coefficient of the nonlinear term is rational, new parametric representations are obtained for the solution of the boundary value problem on the half-line and on the interval. For the problem on the half-line, a new efficient formula is given for the first term of the well-known Coulson–March expansion of the solution in a neighborhood of infinity, and generalizations of this representation and its analogues for the inverse of the solution are obtained. For the Thomas–Fermi model of a multielectron atom and a positively charged ion, highly efficient computational algorithms are constructed that solve the problem for an atom (that is, the boundary value problem on the half-line) and find the derivative of this solution with any prescribed accuracy at an arbitrary point of the half-line. The results are based on an analytic property of a special Abel equation of the second kind to which the original Emden–Fowler equation reduces, to be precise, the property of partially passing a modified Painlevé test at a nodal singular point.

Keywords: Emden–Fowler equation, Thomas–Fermi problem, parametric representation, Abel equation of the second kind, Painlevé test, Fuchs index

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1. INTRODUCTION

1.1. Thomas–Fermi Model

According to the Thomas–Fermi model of a multielectron atom or an ion at the absolute zero temperature (see [1; 2; 3, Section 70]), the dimensionless spatial charge density obeys the nonlinear equation

$$\Delta\Phi(\mathbf{x}) = \frac{8\sqrt{2}}{3\pi}\Phi^{3/2}(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3\backslash\{0\}, \tag{1.1}$$

where Δ is the Laplace operator in в $\mathbb{R}^3$. In the spherically symmetric case, with allowance for the natural requirements for the behavior of Φ at infinity and near a point nucleus (that is, as $|\mathbf{x}| \to 0$), model (1.1) leads to the following boundary value problem for a singular second-order ordinary differential equation:

$$\frac{d^2\Psi}{dr^2} - \frac{1}{\sqrt{r}}\Psi^{3/2}(r) = 0, \quad r \in (0, R), \tag{1.2}$$

$$\lim_{r\to+0}\Psi(r) = Z, \quad \lim_{r\to R}\Psi(r) = 0, \tag{1.3}$$

where $r = \mathrm{const}|\mathbf{x}|$ is the dimensionless distance to the nucleus with charge $+Z$, $R \in (0, +\infty)$ is the ion radius ($R = +\infty$ for an atom), and the screening coefficient $\Psi = \Psi(r)$ specifies the intra-atomic electrostatic potential by the formula $\Phi = \Psi/|\mathbf{x}|$. The total ion charge Z', $0 < Z' < Z$, can be found within this model using the formula

$$Z' = -R\frac{d\Psi}{dr}(R). \tag{1.4}$$

Figure 1 shows plots of solutions of problem (1.2), (1.3) with $Z = 1$ and various values of R.

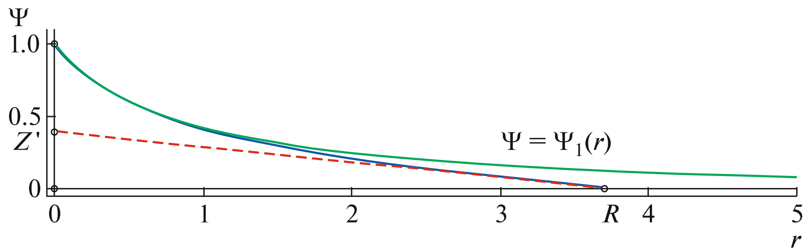

Fig. 1. Plots of solutions of problem (1.2), (1.3) with $Z = 1$ simulating the Thomas–Fermi atom ($R = +\infty$) and a positively charged ion ($R < +\infty$).

Note that the basic principles of the Thomas–Fermi model are used in simulating an inhomogeneous electron gas within the so-called density functional method (see [4]).

1.2. Emden–Fowler Equation and Some Properties of Its Solutions

We consider the following two-point boundary value problem for the Emden–Fowler equation (see [5, Ch. VIII]):

$$\frac{d^2y}{dr^2} - r^{\nu} y^{1+\sigma}(r) = 0, \quad r \in (0, R), \quad R \in (0, +\infty], \quad \nu > -1, \quad \sigma > 0, \tag{1.5}$$

$$\lim_{r \to +0} y(r) = Z, \quad Z \in (0, +\infty), \tag{1.6}$$

$$\lim_{r \to R} y(r) = 0, \tag{1.7}$$

where R and Z are some given numbers. Note that (1.2), (1.3) is a particular case of problem (1.5)–(1.7) with parameter values of $\nu = -1/2$ and $\sigma = 1/2$.

It is well known (see [5, 6]) that with $0 < R \le +\infty$ and $Z \in (0, +\infty)$, problem (1.5)–(1.7) has a unique classical solution being a monotonically decreasing positive analytic function on the interval $r \in (0, R)$. It is also well known (see [5, Ch. VII, Section 7]) that each positive solution $y(r)$ of Eq. (1.5) with $\nu > -2$ defined on the half-line $\{r > 0\}$ has the asymptotic form

$$y(r) \sim f_0^{1/\sigma} r^{-\beta}, \quad r \to +\infty, \tag{1.8}$$

where

$$\beta := \frac{\nu + 2}{\sigma} > 0, \quad f_0 := \beta(\beta + 1) > 0. \tag{1.9}$$

In addition, Eq. (1.5) is invariant with respect to the change of variables

$$\forall \varkappa > 0: \quad r \mapsto (\varkappa r), \quad y \mapsto (\varkappa^{-\beta} y). \tag{1.10}$$

In the particular case of Thomas–Fermi problem (1.2), (1.3), parameters (1.9) assume values of $\beta = 3$ and $f_0 = 12$; scaling formula (1.10) makes it possible (see [2, 7]) to express the solution $\Psi(r)$ of this problem in terms of the solution $\Psi_1(r)$ of the same problem with $Z = 1$ in the form

$$\Psi(r) = Z\Psi_1(Z^{-1/3} r).$$

In connection with this, $\Psi_1(r)$ is said to be the standard solution of the Thomas–Fermi problem for a neutral atom (see [8, Section 172]). Note that the solution of general problem (1.5)–(1.7) is given by a similar formula

$$y(r) = Zy_1(Z^{-1/\beta} r). \tag{1.11}$$

With negative values of $\nu \in (-1, 0)$, the left-hand endpoint $r = 0$ of the interval $r \in [0, R]$ considered in problem (1.5)–(1.7) is a singular point of the equation, since the coefficient of the nonlinear term is infinite. Regarding problem (1.2), (1.3), it is well known (see [9]) that for any $R \in (0,+\infty]$, its solution can be represented in a neighborhood of $r = 0$ by a convergent Puiseux series in powers of $\sqrt{r}$:

$$\Psi(r) = Z + b_2 r + b_3 r^{3/2} + \ldots; \tag{1.12}$$

solutions with a fixed Z and distinct R have distinct values of the slope of the plot at zero $\Psi'(0) = b_2 \in (-\infty, B]$, where $B = B(Z)$ is some negative number. The coefficients b_k, $k \geq 3$, are uniquely determined by Z and b_2 from Eq. (1.2) (see [10]). The solution of problem (1.2), (1.3) on the semi-infinite interval ($R = +\infty$) is associated with the critical value $b_2 = B(Z)$ in expansion (1.12), which is

$$B(1) = \frac{d\Psi_1}{dr}(0) = -1.5880710226\ldots \tag{1.13}$$

at $Z = 1$. Note that the quantity b_2 in the Thomas–Fermi model has the following physical meaning: up to a factor, this is the energy of the Coulomb interaction of the electron cloud with the nucleus (see [8, Section 174]).

It is well known that the solution of problem (1.2), (1.3) with $R = +\infty$ can be approximately obtained in a neighborhood of infinity using the formula (the so-called Coulson–March expansion, see [11, 12]):

$$\Psi(r) = 12^2 r^{-3} \sum_{k=0}^{\infty} a_k (rZ^{1/3})^{\alpha k}, \quad \alpha = \frac{7-\sqrt{73}}{2}, \quad a_0 = 1, \quad a_1 = A := -13.76\ldots, \tag{1.14}$$

where each of the coefficients a_k, $k \geq 2$, can be explicitly expressed in terms of $a_0, \ldots, a_{k-1}$ by recurrence-type formulas.

An extensive literature is devoted to finding numerical values of critical slope (1.13) in expansion (1.12) and the constant A in expansion (1.14), as well as to developing methods to solve problem (1.2), (1.3) (see [1, 2, 7, 10–45]).

1.3. Description of the Results

To formulate the results of this study, we introduce constants ω_0 and α depending only on the parameters ν and σ of Eq. (1.5) by the formulas

$$\omega_0 := -(2\beta + 1) < 0, \tag{1.15}$$

$$\alpha := -\frac{\omega_0 + \sqrt{\omega_0^2 + 4\sigma f_0}}{2} < 0, \tag{1.16}$$

where the numbers β and f_0 are defined in (1.9). If ν in Eq. (1.5) is a rational number, then we represent it as an irreducible fraction

$$\nu =: \frac{N}{M} > -1, \quad N \in \mathbb{Z}, \quad M \in \mathbb{N}. \tag{1.17}$$

The main result (Theorem 1) consists in the following parametric representation of the solution of problem (1.5)–(1.7), (1.17) with $R = +\infty$:

$$r(t) = T_1 t^{1/\alpha}(1-t)^M \mathcal{H}(t), \quad y(t) = T_2 t^{-\beta/\alpha} \mathcal{H}^{-\beta}(t), \quad t \in (0,1], \tag{1.18}$$

where β and α are given by (1.9) and (1.16), respectively, $T_1, T_2 = \text{const} > 0$, and the function $\mathcal{H}(t)$ is positive and analytic on the whole of the interval $t \in [0,1]$, including its endpoints. Note that a parameter value of $t = 0$ corresponds to the limit as $r \to +\infty$, $y \to 0$, while $t = 1$ corresponds to $r = 0$, $y = Z$. We have derived recurrence-type formulas for coefficients of the Taylor series of the function $\mathcal{H}(t)$ in a neighborhood of $t = 0$ and proposed a method to calculate the Taylor series expansion at interior points of the interval $t \in [0,1]$.

Representation (1.18) develops the well-known approach (see [38–45]) to constructing the solution of the Thomas–Fermi problem in a parametric form. We also note an analytical numerical method constructed in [46, Sections 4 and 5] to solve a singular boundary value problem for a nonlinear singularly perturbed equation similar to Eq. (1.5). The novelty of the approach of this work lies in using a previously established analytic property (see [47]) of a special second-kind Abel equation to which the original

Emden–Fowler equation reduces, to be precise, the property of partially passing a modified Painlevé test (see [48]) at a nodal singular point.

The method of solving problem (1.2), (1.3) based on representation (1.18) (with $M = 2$, $N = -1$, $\beta = 3$, and $\alpha = (7 - \sqrt{73})/2$) combines a high accuracy of results and a relatively small computational complexity, which is difficult to achieve within previously proposed methods. This combination is based on the fact that the Taylor series of the function $\mathcal{H}(t)$ at $t = 0$ has an exponentially fast convergence rate for the whole of the interval $t \in [0,1]$ (the empirical value of the convergence radius is ≈ 1.2; a theoretical lower bound for this radius is also given in this study), which makes it possible to efficiently find the solution $\Psi(r)$ and its derivative $\Psi'(r)$ at an arbitrary point of the half-line $r \in [0,+\infty)$ with almost any predetermined accuracy.

In this work, we have also obtained (see Theorem 5) a representation of type (1.18) for the solution of two-point boundary value problem (1.5)–(1.7) on the finite interval $[0, R]$ with $R \in (0,+\infty)$ and $Z \in (0,+\infty)$. This problem statement within the Thomas–Fermi model corresponds to the case of a positively charged ion.

A consequence of the parametric formulas derived by us (see Theorem 6) is the representability of the solution of problem (1.5)–(1.7) with $R \in (0,+\infty]$, $Z > 0$, and a rational ν as a convergent series

$$y(r) = Z + b_M r + b_{M+1} r^{1+1/M} + b_{M+2} r^{1+2/M} + \ldots \tag{1.19}$$

in powers of $r^{1/M}$, where M is defined by (1.17), in a neighborhood of $r = 0$. Note that when condition (1.17) is violated and also when $\nu \le -1$, the analytic structure of the solution $y(r)$ in a neighborhood of $r = 0$ can be more complicated than representation (1.19) (see [49, Section 12.4]).

Like in the case of expansion (1.12), which is generalized by (1.19), the value of $b_M \in (-\infty, B]$ parametrizes the solution of problem (1.5)–(1.7) with a given Z and distinct $R \in (0,+\infty]$; here, $B = B(Z,\sigma,\nu)$ is the slope of the plot at zero for the solution of the problem on the semi-infinite interval, that is, with $R = +\infty$. It follows from (1.11) that

$$B(Z,\sigma,\nu) = Z^{1+1/\beta} B(1,\sigma,\nu).$$

In this work, we have derived a formula (see (2.15)) for the critical value $B(1,\sigma,\nu)$ of the derivative of the solution at zero with $Z = 1$, which generalizes the well-known Majorana formula (see [40]) for quantity (1.13). In connection with this, we note an analytical numerical method constructed in [50, 51] to find the Blasius constant, which arises in boundary layer theory.

Theorem 2 of this work gives the following representation of the solution of problem (1.5)–(1.7), $R = +\infty$, in a neighborhood of $r = +\infty$, which generalizes expansion (1.14) and improves asymptotics (1.8):

$$y(r) = f_0^{1/\sigma} r^{-\beta} \sum_{n=0}^{\infty} a_n (Z^{1/\beta} r)^{n\alpha}, \quad a_0 = 1, \quad a_1 = a_1(\sigma,\nu), \tag{1.20}$$

where the coefficients a_n do not depend on Z and β and α are given by (1.9) and (1.16), respectively. A formula is obtained for $a_1(\sigma,\nu)$ (see (2.43)), which makes it possible to find the constant A in (1.14) with any predetermined accuracy (see (3.5)).

It is well known (see [52]) that expansion (1.14) converges only for sufficiently large r. Theorems 3 and 4 give new representations similar to (1.20) and (1.14) for the inverse $r(y)$ of the solution $y(r)$:

$$r(y) = \frac{f_0^{1/(\nu+2)}}{y^{1/\beta}} \sum_{n=0}^{\infty} A_n (y/Z)^{-n\alpha/\beta}, \tag{1.21}$$

$$r(y) = \frac{f_0^{1/(\nu+2)}}{y^{1/\beta}} \sum_{n=0}^{\infty} A_n' \mathcal{Y}^n, \quad \mathcal{Y} := 1 - \sqrt[M]{1 - (y/Z)^{-\alpha/\beta}} \in (0,1]; \tag{1.22}$$

the series in $\mathcal{Y}$ on the right-hand side of the first equality in (1.22) in the case of problem (1.2), (1.3) has an exponentially fast convergence rate for the whole of the interval $\mathcal{Y} \in [0,1]$, that is, with $y \in [0, Z]$, which makes this formula suitable to calculate the solution on the whole of its domain. By approximating the sum of this series by a quadratic function on a unit interval (see Section 3.1), we arrive at

$$r(\Psi) \approx 12^{2/3} \Psi^{-1/3} \left(1 - (\Psi/Z)^{-\alpha/3}\right). \tag{1.23}$$

The analyticity of the function $\mathscr{H}(t)$ in representation (1.18) at $t = 1$ is due to some property of a nodal singular point of the second-kind Abel equation, being an auxiliary first-order equation to which original equation (1.5) is reduced by an order decreasing procedure. This property lies in that the family of solutions of the equation passing through its nodal point at the origin can be specified by a general formula including a series in fractional powers of the variable with one of the coefficients of the series being a parameter of this family. As has been shown in [47], this analytic structure of solutions of the second-kind Abel equation near its nodal singular point is associated with partially passing a modification of the Painlevé test for this equation. Note that new representations of quasi-stationary solutions of nonlinear parabolic Kolmogorov–Petrovskii–Piskunov-type equations were obtained in [53–55] using the above-mentioned property of the second-kind Abel equation.

1.4. Transition to an Autonomous Second-Order Equation

We set

$$I(R) := (-\infty, \ln R), \qquad R \in (0, +\infty], \tag{1.24}$$

where $\ln(+\infty) = +\infty$ by definition. Using notation (1.9), we switch in problem (1.5)–(1.7) to new variables

$$\psi := f_0^{-1/\sigma} r^{\beta} y(r) > 0, \qquad \rho := \ln r \in I(R), \tag{1.25}$$

with respect to which original equation (1.5), in view of definition (1.15), takes the autonomous form

$$\frac{d^2\psi}{d\rho^2} + \omega_0 \frac{d\psi}{d\rho} + f_0 \psi(1 - \psi^{\sigma}) = 0. \tag{1.26}$$

Thus, there is a one-to-one correspondence between solutions $y(r)$ of problem (1.5)–(1.7) and solutions $\psi(\rho)$ of Eq. (1.26) defined on an interval $I(R)$ of form (1.24). By inversing (1.25), we arrive at

$$r = \exp\rho, \qquad y = f_0^{1/\sigma} \psi r^{-\beta}. \tag{1.27}$$

We fix a solution $y(r)$ of problem (1.5)–(1.7) with some $0 < R \le +\infty$ and $Z \in (0, +\infty)$ and consider the behavior of the corresponding solution $\psi(\rho)$ of Eq. (1.26). Substitution formula (1.25) and condition (1.6) yield the asymptotics

$$\psi(\rho) = O(e^{\beta\rho}) \quad \text{as} \quad \rho \to -\infty, \tag{1.28}$$

while condition (1.7) and relation (1.8) imply the equality

$$\lim_{\rho \to \ln R} \psi(\rho) = \begin{cases} 0, & R \in (0, +\infty), \\ 1, & R = +\infty. \end{cases} \tag{1.29}$$

Due to the autonomy of Eq. (1.26), its solution $\psi(\rho)$ becomes a solution of the same equation under a shift

$$\rho \mapsto (\rho + \ln \varkappa), \qquad \varkappa > 0, \tag{1.30}$$

along the ρ axis. It can be seen from (1.25) and (1.27) that translation (1.30) corresponds to scale transformation (1.10) of Eq. (1.5). In addition, translation (1.30) preserves the quantity

$$\mu := \sup_{\rho \in I(R)} \psi(\rho) > 0, \tag{1.31}$$

which is thus an invariant of (1.10).

Relying on (1.6) and (1.7), we prove the inclusion

$$\mu \in (0, 1] \tag{1.32}$$

by contradiction. Indeed, the assumption $\mu > 1$ and asymptotics (1.28) and (1.29) imply that the function $\psi(\rho)$ has a local maximum at some point $\rho_0 \in I(R)$, $\psi(\rho_0) > 1$. Then the conditions

$$\frac{d^2\psi}{d\rho^2}(\rho_0) \le 0, \quad \frac{d\psi}{d\rho}(\rho_0) = 0, \quad \psi(1 - \psi^{\sigma}) < 0$$

must be satisfied at this point, which collectively contradict Eq. (1.26). Therefore, the assumption $\mu > 1$ is not valid, and inclusion (1.32) holds.

The following proposition follows directly from Proposition 5 in [47].

Proposition 1. *For each* μ *from half-open interval* (1.32)*, there is a solution* $\psi = \psi_\mu(\rho)$ *of problem* (1.26)–(1.29) *on an interval* $I(R)$ *of form* (1.24) *with some* $R \in (0,+\infty]$ *such that relation* (1.31) *holds for* μ. *The function* $\psi_\mu(\rho)$ *is uniquely defined up to translation* (1.30)*;* $\mu = 1$ *if and only if* $R = +\infty$.

The above reasoning and Proposition 1 yield the following proposition.

Proposition 2. *The set of solutions* $y(r)$ *of problem* (1.5)–(1.7)*,* $Z \in (0,+\infty)$*,* $R \in (0,+\infty]$*, is in a one-to-one correspondence with the set of solutions of problem* (1.26)–(1.29)*,* (1.31)*,* (1.32) *with* $\mu \in (0,1]$. *This correspondence, given by* (1.25) *and* (1.27)*, is consistent with transformations* (1.10) *and* (1.31) *so that interval* (1.32) *parametrizes equivalence classes of solutions* $y(r)$ *with respect to scaling* (1.10).

In what follows, it is convenient to specify a solution $y(r)$ of problem (1.5)–(1.7) not by a pair (R, Z), where $R \in (0,+\infty]$ and $Z \in (0,+\infty)$, but by a pair (μ, Z), where $\mu \in (0,1]$ and $Z \in (0,+\infty)$.

1.5. Decreasing the Equation Order and a Condition for Passing the Painlevé Test

We define a new variable $p = p(\psi)$ as

$$p(\psi) := \frac{d\psi}{d\rho}; \tag{1.33}$$

then problem (1.26), (1.28), (1.29), (1.31) with $\mu \in (0,1]$ reduces to the following (singular) Cauchy problem with respect to $p(\psi)$:

$$p(\psi)\frac{dp}{d\psi} + \omega_0 p(\psi) + f_0\psi(1-\psi^\sigma) = 0, \quad p(\mu) = 0. \tag{1.34}$$

We define the Fuchs index for the nodal point $\psi = 0$, $p = 0$ of Eq. (1.34), in view of (1.9) and (1.15), as follows:

$$K := -\frac{\omega_0 + 2\beta}{\beta\sigma} = \frac{1}{\sigma\beta} = \frac{1}{\nu+2}. \tag{1.35}$$

If condition (1.17) is satisfied and thus $K \in \mathbb{Q} \cap (0,1)$, then, according to [47, Section 2.3], Eq. (1.34) partially passes a modified Painlevé test. In this case, let $\tilde{N}$ denote the denominator of the fraction representing K:

$$K =: \frac{M}{\tilde{N}} \in \mathbb{Q} \cap (0,1), \quad \tilde{N} = N + 2M > M. \tag{1.36}$$

We introduce variables q and z related to p and ψ as follows:

$$p =: \psi q, \quad \psi =: z^{\tilde{N}/\sigma}; \tag{1.37}$$

then problem (1.34) with respect to $q(z)$ assumes the form

$$\frac{\sigma}{2\tilde{N}} z\frac{dq^2}{dz} + q^2(z) + \omega_0 q(z) + f_0(1 - z^{\tilde{N}}) = 0, \tag{1.38}$$

$$q\left(\mu^{\sigma/\tilde{N}}\right) = 0, \quad \mu \in (0,1]. \tag{1.39}$$

According to Proposition 1 in [47], all trajectories representing solutions of problem (1.34) on the (ψ, p) plane arrive at the origin $\psi = 0$, $p = 0$ with the slope β to the horizontal and the corresponding solutions of problem (1.38), (1.39) have the property $q(0) = \beta$. We apply Theorem 1 from [47] to deduce the following proposition.

Proposition 3. *Each solution* $q(z)$ *of Eq.* (1.38) *with the condition* $q(0) = \beta$ *is an analytic function at* $z = 0$ *of the form*

$$q(z) = \beta\left(1 + z^M \mathfrak{Q}(z)\right), \tag{1.40}$$

where the function $\mathfrak{Q}(z)$ *is also analytic at* $z = 0$. *Solutions* (1.40) *form a family parametrized by* $C := \mathfrak{Q}(0)$, *that is, for each* $C \in \mathbb{R}$ *there is a unique solution* $q(z)$ *of form* (1.40). *Coefficients of the Taylor series of* $\mathfrak{Q}(z)$ *at* $z = 0$ *can be rationally expressed in terms of* β, M, $\tilde{N}$, *and* C.

Solutions $q = q_\mu(z)$ *of problem* (1.38), (1.39) *with* $\mu \in (0,1]$ *belong to this family, and formula* (1.40) *defines the function* $\mathfrak{Q} = \mathfrak{Q}_\mu(z)$ *for each* $\mu \in (0,1]$. *The mapping*

$$(0,1] \ni \mu \mapsto C(\mu) := \mathfrak{Q}_\mu(0) \in (-\infty, C_1], \quad C_1 := C(1) = \mathfrak{Q}_1(0) < 0,$$

is monotonic and bijective.

Thus, Proposition 3 asserts that when condition (1.17) is satisfied, changing to variables z, $\mathfrak{Q}$ in Abel equation (1.34) eliminates in a certain sense the irregularity of this equation at the nodal point $\psi = 0$, $p = 0$.

2. PARAMETRIC REPRESENTATION OF THE SOLUTION OF THE EMDEN–FOWLER EQUATION

2.1. Solution of the Problem on the Semi-Infinite Interval

We consider problem (1.5)–(1.7), $R = +\infty$, with some $Z > 0$. Due to Propositions 1 and 2, its solution $y(r)$ can be expressed by formulas (1.27) in terms of the solution $\psi = \psi_1(\rho)$ of problem (1.26), (1.28), (1.29), (1.31) with $\mu = 1$.

2.1.1. Parametric representation of the solution and its derivative. Assume that ν in Eq. (1.5) satisfies rationality condition (1.17). Then Theorem 2 in [47] asserts that the function $\psi = \psi_1(\rho)$ has the parametric representation

$$\psi = (1-t)^{\tilde{N}/\sigma}, \quad \rho = M\ln(1-t) + \frac{1}{\alpha}\ln t + H(t), \quad t \in (0,1), \tag{2.1}$$

where $\tilde{N}$ is defined by (1.36); $H(t)$ is an analytic function on the interval $t \in [0,1]$ and can be expressed using the formulas

$$H(t) = \int_0^t h(t)\,dt, \quad h(t) = -\frac{1}{\alpha t} + M\mathfrak{Q}(t)\frac{(1-t)^{M-1}}{1+(1-t)^M\mathfrak{Q}(t)} \tag{2.2}$$

in terms of the solution $\mathfrak{Q}(t)$ of the Cauchy problem

$$\frac{d\mathfrak{Q}}{dt} = -(\beta+1)M\frac{(1-t)^{M-1}\mathfrak{Q}^2(t) - (1-t)^{\tilde{N}-M-1}}{1+(1-t)^M\mathfrak{Q}(t)}, \quad t \in [0,1], \tag{2.3}$$

$$\mathfrak{Q}(0) = -1, \quad \frac{d\mathfrak{Q}}{dt}(0) = -(\alpha+1)M. \tag{2.4}$$

Here, $\mathfrak{Q}(t)$ is a decreasing negative analytic function on the interval $t \in [0,1]$ and the function

$$g(t) := 1 + (1-t)^M\mathfrak{Q}(t), \quad t \in [0,1], \tag{2.5}$$

which enters the denominator on the right-hand side of Eq. (2.3), is nonnegative and increasing on the unit interval, $g(0) = 0$, $g(1) = 1$. The variable t is related to z in (1.37) by the equality

$$t + z = 1, \tag{2.6}$$

and $g(t) = \beta^{-1}q(t)$, where $q(t)$ has form (1.40).

Upon substituting parametrization (2.1) into (1.27), in view of the equality

$$\frac{\tilde{N}}{\sigma} - \beta M = 0, \tag{2.7}$$

which is implied by (1.35) and (1.36), we derive representation (1.18), where $T_1 = \text{const} > 0$,

$$\mathcal{H}(t) := \exp H(t), \tag{2.8}$$

$$T_2 = f_0^{1/\sigma}T_1^{-\beta}. \tag{2.9}$$

We choose the constant T_1 in (2.1) so that boundary condition (1.6) be satisfied. Upon introducing the notation

$$\mathcal{H}_e := \mathcal{H}(1), \tag{2.10}$$

substituting $t = 1$ into (1.18), and equating the resulting expression for y at $r = 0$ to Z, we write condition (1.6) in the form

$$f_0^{1/\sigma} T_1^{-\beta} \mathcal{H}_e^{-\beta} = Z.$$

In view of (2.9), this yields

$$T_1 = \frac{f_0^K}{\mathcal{H}_e} Z^{-1/\beta}, \quad T_2 = \mathcal{H}_e^{\beta} Z, \tag{2.11}$$

where K is specified by (1.35).

Based on (2.2), (2.8), and (2.5), we find the derivatives of the functions $r(t)$ and $y(t)$ in parametric representations (1.18) in the form

$$\frac{dy}{dt} = y(t)\frac{d\ln y}{dt} = -\beta y(t)\frac{d}{dt}\left(\frac{1}{\alpha}\ln t + H(t)\right) = -\beta\left(\frac{1}{\alpha t} + h(t)\right)y(t) = -\beta M\frac{(1-t)^{M-1}\mathcal{Q}(t)}{g(t)}y(t), \tag{2.12}$$

$$\begin{aligned}\frac{dr}{dt} &= r(t)\frac{d\ln r}{dt} = r(t)\frac{d}{dt}\left(M\ln(1-t) + \frac{1}{\alpha}\ln t + H(t)\right) = \left(-\frac{M}{1-t} + \frac{1}{\alpha t} + h(t)\right)r(t)\\ &= \left(-\frac{M}{1-t} + M\frac{(1-t)^{M-1}\mathcal{Q}(t)}{1+(1-t)^M\mathcal{Q}(t)}\right)r(t) = -\frac{M}{(1-t)g(t)}r(t).\end{aligned} \tag{2.13}$$

Using (2.12) and (2.13), we calculate the derivative of the solution dy/dr as a function of the parameter $t \in (0,1]$:

$$\frac{dy}{dr} = \frac{dy}{dt}\left(\frac{dr}{dt}\right)^{-1} = \beta\frac{y(t)}{r(t)}(1-t)^M\mathcal{Q}(t) = \beta\frac{T_2}{T_1}t^{-(\beta+1)/\alpha}\mathcal{H}^{-(\beta+1)}(t)\mathcal{Q}(t), \quad t \in (0,1], \tag{2.14}$$

where the constants T_1 and T_2 are specified by (2.11). In particular, relation (2.14) with $t = 1$, in view of (2.10) and (2.11), yields an expression for the critical slope of the plot of $y(r)$ at $r = 0$ of the form

$$\frac{dy}{dr}(0) = \frac{T_2}{T_1}\mathcal{H}_e^{-(\beta+1)}\mathcal{Q}_e = f_0^{-K}Z^{(\beta+1)/\beta}\mathcal{Q}_e, \quad \mathcal{Q}_e := \mathcal{Q}(t)\big|_{t=1}. \tag{2.15}$$

Note that, due to (2.12), (2.13), and (1.18), both derivatives dy/dt and dr/dt have zeros of order $(M-1)$ at $t = 0$ and are nonzero at other points of the unit interval.

2.1.2. Calculating Taylor coefficients and estimating the convergence radius. For the functions $\mathcal{Q}(t)$ and $\mathcal{H}(t)$ introduced above in (2.2)–(2.4), (2.8), we calculate coefficients of the expansions in powers of t. Using notation (2.5), we rewrite Eq. (2.3) in the form

$$g(t)\frac{d\mathcal{Q}}{dt} = (\beta+1)M\left((1-t)^{M-1}\mathcal{Q}^2(t) - (1-t)^{\tilde{N}-M-1}\right), \quad t \in [0,1], \tag{2.16}$$

and substitute the formal expansions

$$\mathcal{Q}(t) =: \sum_{n=0}^{\infty}\mathcal{Q}_n t^n, \quad \mathcal{Q}_0 = -1, \quad \mathcal{Q}_1 = -(\alpha+1)M, \tag{2.17}$$

$$g(t) =: \sum_{n=1}^{\infty} g_n t^n, \quad g_n = \sum_{j=0}^{M}(-1)^j\binom{M}{j}\mathcal{Q}_{n-j}, \quad n \ge 1, \quad g_1 = -\alpha M, \tag{2.18}$$

into system (2.5), (2.16).

Upon equating the coefficients of t^n, $n \ge 2$, on both sides of (2.16), we arrive at

$$\sum_{j=1}^{n} j\mathcal{Q}_j g_{n-j+1} = (\beta+1)M\left[\sum_{j,k=0}^{n}(-1)^{n-j-k}\binom{M-1}{n-j-k}\mathcal{Q}_j\mathcal{Q}_k + (-1)^{n+1}\binom{\tilde{N}-M-1}{n}\right].$$

We rewrite the last equality in the form

$$\mathcal{Q}_1\mathcal{Q}_n + n\mathcal{Q}_n g_1 - 2(\beta+1)M\mathcal{Q}_0\mathcal{Q}_n = V_n, \tag{2.19}$$

where the right-hand side

$$V_n := (\beta+1)M\left[\sum_{j,k=0}^{n-1}(-1)^{n-j-k}\binom{M-1}{n-j-k}\mathfrak{Q}_j\mathfrak{Q}_k + (-1)^{n+1}\binom{\tilde{N}-M-1}{n}\right] - \mathfrak{Q}_1\sum_{j=1}^{M}(-1)^j\binom{M}{j}\mathfrak{Q}_{n-j} - \sum_{j=2}^{n-1} j\,\mathfrak{Q}_j g_{n-j+1} \tag{2.20}$$

depends only on $\mathfrak{Q}_j$, g_j, $j = 0, \ldots, (n-1)$, and does not depend on $\mathfrak{Q}_n$. We find the factor of $\mathfrak{Q}_n$ on the left-hand side of (2.19):

$$\begin{gathered}\mathfrak{Q}_1 + ng_1 - 2(\beta+1)M\mathfrak{Q}_0 = -(\alpha+1)M - n\alpha M + 2(\beta+1)M \\ = -\left(\alpha(n+1)+1-2(\beta+1)\right)M = -\left((n+1)\alpha+\omega_0\right)M > 0, \quad n \geq 2.\end{gathered} \tag{2.21}$$

We solve (2.19) as a linear equation with respect to $\mathfrak{Q}_n$ successively with $n = 2, 3, \ldots$ and, in view of (2.21), obtain

$$\mathfrak{Q}_n = \frac{V_n}{-\left(\omega_0 + (n+1)\alpha\right)M}, \quad n \geq 2. \tag{2.22}$$

Formulas (2.18), (2.20), and (2.22) make it possible to calculate each of the coefficients of Taylor series expansion (2.17) of $\mathfrak{Q}(t)$ in a finite number of arithmetic operations.

We find coefficients of the Taylor series

$$h(t) =: \sum_{n=0}^{\infty} h_n t^n \tag{2.23}$$

of $h(t)$ based on (2.2), (2.5), and (2.7):

$$\begin{gathered}h(t) = -\frac{1}{\alpha t} + \frac{M(1-t)^{M-1}\mathfrak{Q}(t)}{g(t)} = \frac{M(1-t)^{M-1}\mathfrak{Q}(t) - \alpha^{-1}t^{-1}g(t)}{g(t)} \\ = \frac{t^{-1}\left(M(1-t)^{M-1}\mathfrak{Q}(t) - \alpha^{-1}t^{-1}g(t)\right)}{t^{-1}g(t)}.\end{gathered} \tag{2.24}$$

Upon substituting expansions (2.17) and (2.18) into (2.24), we arrive at

$$\left(\sum_{n=0}^{\infty} h_n t^n\right) \times \left(\sum_{n=0}^{\infty} g_{n+1} t^n\right) = \sum_{n=0}^{\infty} G_n t^n,$$

where G_n is the coefficient of t^n in the numerator of fraction (2.24):

$$G_n = -\frac{g_{n+2}}{\alpha} + M\sum_{j=0}^{n+1}(-1)^j\binom{M-1}{j}\mathfrak{Q}_{n+1-j}, \quad n \geq 0, \tag{2.25}$$

which yields

$$h_n = \frac{1}{g_1}\left(G_n - \sum_{j=0}^{n-1} h_j g_{n+1-j}\right), \quad n \geq 0. \tag{2.26}$$

For Taylor coefficients H_n of the function

$$H(t) = \int_0^t h(t)\,dt =: \sum_{n=1}^{\infty} H_n t^n, \tag{2.27}$$

we have

$$H_n = \frac{h_{n-1}}{n}, \quad n \geq 1. \tag{2.28}$$

To obtain the Taylor series for (2.8), we expand brackets and combine like terms on the right-hand side of the formula

$$\mathcal{H}(t) = \exp H(t) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \left(\sum_{k=0}^{\infty} H_{k+1} t^k \right)^n, \tag{2.29}$$

where the coefficient of t^n is a polynomial of $H_1, \ldots, H_n$.

To estimate the convergence radius for series (2.17), (2.18), and (2.23), we additionally assume that the parameter σ in (1.5) is in the range

$$\sigma \in (0,1]. \tag{2.30}$$

We first show that the solution $p = p_1(\psi)$ of problem (1.34), $\mu = 1$, is an analytic function in the disc $\mathbb{C} := \{|\psi - 1| < 1\}$. Due to Proposition 4 in [47], it suffices to show that the free term $F(\psi) = f_0 \psi(1 - \psi^{\sigma})$ of this equation has the following properties: first, $F(\psi)$ is a holomorphic function inside $\mathbb{C}$ that is nonzero everywhere in the disc except for its center $\psi = 1$; second, coefficients of the expansion of the function $F(\psi)/\psi$ at $\psi = 1$ in powers of the variable $\tau := (1 - \psi)$ form a decreasing sequence of positive numbers. The first condition is obviously satisfied. We verify the second condition:

$$f_0(1 - \psi^{\sigma}) = f_0(1 - (1 - \tau)^{\sigma}) = f_0 \sum_{k=1}^{\infty} (-1)^{k+1} \binom{\sigma}{k} \tau^k,$$

which yields the required result in view of condition (2.30).

When the variable ψ is replaced by t using substitutions (1.37) and (2.6), the disc of convergence $\mathbb{C}$ for the function $p_1(\psi)$ is conformly mapped onto a convex drop-shaped domain of analyticity $\mathfrak{D}$ of the functions $\mathfrak{Q}(t)$, $q(t)$, $h(t)$, $H(t)$, and $\mathcal{H}(t)$. The domain $\mathfrak{D}$ has an angular point with the angle opening $(\pi\sigma/\tilde{N})$ at $t = 1$. The distance from the origin $t = 0$ to the boundary $\partial\mathfrak{D}$ is

$$R(\sigma, \tilde{N}) := 2^{\sigma/\tilde{N}} - 1. \tag{2.31}$$

Thus, we have obtained the following result.

Proposition 4. *When condition* (2.30) *is satisfied, the functions* $\mathfrak{Q}(t)$, $q(t)$, $h(t)$, $H(t)$, *and* $\mathcal{H}(t)$ *are holomorphic in the domain* $\mathfrak{D}$ *and quantity* (2.31) *is a lower bound for the convergence radius for series* (2.17), (2.18), *and* (2.23).

When the value of $\mathfrak{Q}(t)$ at some interior point of the unit interval $t \in (0,1)$ is obtained, we can find the Taylor series expansions for $\mathfrak{Q}(t)$ and $g(t)$ at this point by the method of undetermined coefficients from Eqs. (2.5) and (2.16) and then calculate the corresponding expansion for $h(t)$, $H(t)$, and $\mathcal{H}(t)$ using (2.24), (2.27)–(2.29).

We summarize the results obtained in Sections 2.1.1 and 2.1.2 in the following theorem.

Theorem 1. *Consider problem* (1.5)–(1.7), $R = +\infty$, *with* $Z \in (0, +\infty)$ *and condition* (1.17). *Then the solution* $y(r)$ *of this problem and its first derivative* dy/dr *has parametric representations* (1.18), (2.11), *and* (2.14), *that is,*

$$r = T_1 (1 - t)^M t^{1/\alpha} \mathcal{H}(t), \quad t \in (0,1], \quad T_1 = \frac{f_0^{\,K}}{\mathcal{H}_e} Z^{-1/\beta}, \tag{2.32}$$

$$y = T_2 t^{-\beta/\alpha} \mathcal{H}^{-\beta}(t), \quad T_2 = \mathcal{H}_e^{\beta} Z, \tag{2.33}$$

$$\frac{dy}{dr} = T_3 t^{-(\beta+1)/\alpha} \mathcal{H}^{-(\beta+1)}(t) \mathfrak{Q}(t), \quad T_3 = \beta f_0^{\,-K} \mathcal{H}_e^{\beta+1} Z^{(\beta+1)/\beta}, \tag{2.34}$$

where the constants β, f_0, ω_0, α, K, *and* $\mathcal{H}_e$ *depend only on* σ *and* ν *and are specified by* (1.9), (1.15), (1.16), (1.35), *and* (2.10); $\mathcal{H}(t)$ *is a positive analytic function on the interval* $t \in [0,1]$ *and can be expressed in terms of the solution* $\mathfrak{Q}(t)$ *of problem* (2.3), (2.4) *using* (2.24), (2.27), *and* (2.29). *Taylor series expansions* (2.17) *and* (2.29) *for* $\mathfrak{Q}(t)$ *and* $\mathcal{H}(t)$ *at* $t = 0$ *can be obtained using* (2.18), (2.20), (2.22), (2.25)–(2.29). *If* $\sigma \in (0,1]$, *then the convergence radius of these series is bounded from below by* (2.31).

2.1.3. Elimination of the parameter *t*. We consider the solution $y(r)$ of problem (1.5)–(1.7), (1.17), $R = +\infty$, with $Z \in (0, +\infty)$ in form (2.32), (2.33) and eliminate t from this representation. We raise both sides of the equality $\psi = (f_0^{-1/\sigma} r^\beta y)$, that is, of the first formula in (1.25), to the power $\sigma/\tilde{N}$ and write the result, in view of (2.1) and (2.7), in the form

$$r^{1/M} y^{\sigma/\tilde{N}} = f_0^{1/\tilde{N}}(1-t). \tag{2.35}$$

We express t in terms of r using (2.32). We divide both sides of (2.32) by T_1 and raise them to the power α; let $\tilde{r}$ and ξ denote the transformed left- and right-hand sides, respectively:

$$\tilde{r} = \tilde{r}(r) := \left(\frac{r}{T_1}\right)^\alpha = (1-t)^{M\alpha} t \mathcal{H}^\alpha(t) =: \xi(t), \quad t \in [0,1], \quad r, \tilde{r} \in [0,+\infty], \tag{2.36}$$

where $\xi = \xi(t)$ is an analytic function with respect to t on the unit half-open interval.

We verify that $d\xi/dt \neq 0$ for $t \in [0,1)$. Indeed, due to (2.13), in view of (2.5), we have

$$\frac{d\xi}{dt} = \xi(t)\frac{d\ln\xi}{dt} = \alpha\xi(t)\frac{d\ln r(t)}{dt} = -\frac{M\alpha\xi(t)}{(1-t)g(t)} = -M\alpha(1-t)^{M\alpha-1}\frac{t}{g(t)}\mathcal{H}^\alpha(t) > 0.$$

Therefore, the correspondence $t \mapsto \tilde{r} = \xi(t)$ specified by (2.36) monotonically and bijectively maps the interval $t \in [0,1)$ onto the ray $\tilde{r} \in [0,+\infty)$. Then there exists the inverse $\theta = \theta(\tilde{r})$ of $\xi(t)$, being an increasing positive analytic function mapping the half-line $\tilde{r} \in [0,+\infty)$ onto the interval $t \in [0,1)$; thus, the parameter t in (2.32), in view of relation (2.36) between $\tilde{r}$ and r, can be expressed in terms of r in the form

$$t = \theta(\tilde{r}(r)). \tag{2.37}$$

We calculate the expansion of $\xi(t)$ in powers of t. In a neighborhood of $t = 0$, the formulas

$$\begin{aligned}(1-t)^{M\alpha} &= \sum_{n=0}^{\infty}(-1)^n \binom{M\alpha}{n} t^n = 1 - M\alpha t + \ldots, \\ t\mathcal{H}^\alpha(t) &= \sum_{n=0}^{\infty}\frac{t^{n+1}}{n!}\left(\alpha\sum_{k=0}^{\infty}H_{k+1}t^k\right)^n = t + \alpha H_1 t^2 + \ldots\end{aligned} \tag{2.38}$$

are valid; multiplying these, we arrive at

$$\xi(t) = t - \alpha(H_1 - M)t^2 + \cdots := \sum_{n=1}^{\infty}\xi_n t^n, \tag{2.39}$$

$$\theta(\tilde{r}) = \tilde{r} + \alpha(H_1 - M)\tilde{r}^2 + \cdots := \sum_{n=1}^{\infty}\theta_n \tilde{r}^n, \tag{2.40}$$

where the coefficients ξ_n and θ_n polynomially depend on the known quantities α, M, $H_1, \ldots, H_{n-1}$.

Substituting expression (2.37) for t into (2.35), we derive the following representations of the function $y = y(r)$:

$$y^{\sigma/\tilde{N}} = \frac{f_0^{1/\tilde{N}}}{r^{1/M}}(1-\theta(\tilde{r})), \quad y(r) = \frac{f_0^{1/\sigma}}{r^\beta}(1-\theta(\tilde{r}))^{\tilde{N}/\sigma}, \quad \tilde{r} = \tilde{r}(r) \in (0,+\infty); \tag{2.41}$$

in view of (2.40), representation (2.41) in a neighborhood of $r = +\infty$ takes form (1.20):

$$y(r) = \frac{f_0^{1/\sigma}}{r^\beta}\left(1 - \sum_{n=1}^{\infty}\theta_n(rZ^{1/\beta}f_0^{-K}\mathcal{H}_e)^{n\alpha}\right)^{\tilde{N}/\sigma} =: \frac{f_0^{1/\sigma}}{r^\beta}\sum_{n=0}^{\infty}a_n(rZ^{1/\beta})^{n\alpha}, \tag{2.42}$$

$$a_0 = 1, \quad a_1 = -\frac{\tilde{N}}{\sigma f_0^{\alpha K}}\mathcal{H}_e^\alpha. \tag{2.43}$$

We have thus deduced the following theorem.

Theorem 2. *Under the assumptions of Theorem* 1, *the parameter* $t \in (0,1]$ *can be expressed in terms of* r *in form* (2.37). *The solution* $y(r)$ *of problem* (1.5)–(1.7), $R = +\infty$, *has representation* (2.41), *which takes form* (2.42), (2.43) *in a neighborhood of* $r = +\infty$.

We now express t in terms of y from (2.33). Raising both sides of this equality to the power $-\alpha/\beta$ and introducing, by analogy with (2.36), the notation $\tilde{y}$ and Ξ, we obtain

$$\tilde{y} = \tilde{y}(y) := \left(\frac{y}{\mathcal{H}_e^{\beta} Z}\right)^{-\alpha/\beta} = t\mathcal{H}^{\alpha}(t) =: \Xi(t). \tag{2.44}$$

Due to (2.44), (2.12), (2.5), and (1.18), for $t \in [0,1]$ we have

$$\frac{d\Xi}{dt} = \Xi(t)\frac{d\ln\Xi}{dt} = t\mathcal{H}^{\alpha}(t)\left(-\frac{\alpha}{\beta}\frac{d\ln y(t)}{dt}\right) = M\alpha\frac{t}{g(t)}(1-t)^{M-1}\mathfrak{Q}(t)\mathcal{H}^{\alpha}(t);$$

therefore, the derivative $d\Xi/dt$ is positive for $t \in (0,1]$ and has a zero of order $(M-1)$ at $t = 0$. Thus, the mapping $t \mapsto \tilde{y} = \Xi(t)$ defined by (2.44) is a one-to-one correspondence (due to monotonicity) between the intervals $t \in [0,1]$ and $\tilde{y} \in [0, \mathcal{H}_e^{\alpha}]$; consequently, there exists the inverse $\Theta = \Theta(\tilde{y})$ of $\Xi(t)$, being an increasing analytic function on the interval $\tilde{y} \in [0, \mathcal{H}_e^{\alpha})$ and having (as a function of the complex variable $\tilde{y}$) an M-sheeted branching at $\tilde{y} = \mathcal{H}_e^{\alpha}$. Using $\Theta(\tilde{y})$, we express t in terms of y in the form

$$t = \Theta(\tilde{y}(y)). \tag{2.45}$$

The function $\Xi(t)$ has expansion (2.38) in a neighborhood of $t = 0$, which yields a Taylor series expansion of the inverse function at $\tilde{y} = 0$:

$$\Theta(\tilde{y}) = \tilde{y} - \alpha H_1\tilde{y}^2 + \cdots =: \sum_{n=1}^{\infty}\Theta_n\tilde{y}^n. \tag{2.46}$$

Upon substituting t in form (2.45) into formula (2.35) and solving it with respect to r, we derive

$$r^{1/M} = \frac{f_0^{1/\tilde{N}}}{y^{\sigma/\tilde{N}}}(1 - \Theta(\tilde{y}(y))), \tag{2.47}$$

which implies, in view of (2.46), representation (1.21) in a neighborhood of $r = 0$, that is,

$$r(y) = \frac{f_0^{K}}{y^{1/\beta}}\left(1 - \sum_{n=1}^{\infty}\Theta_n\tilde{y}^n\right)^{M} =: \frac{f_0^{K}}{y^{1/\beta}}\sum_{n=0}^{\infty}A_n(y/Z)^{-n\alpha/\beta}, \quad A_0 = 1, \quad A_1 = -M\mathcal{H}_e^{\alpha}. \tag{2.48}$$

Thus, the following theorem is true.

Theorem 3. *Under the assumptions of Theorem* 1, *the parameter* $t \in (0,1]$ *can be expressed in terms of* y *in form* (2.45)*; the function* $t = t(y)$ *has an* M*-sheeted branching at* $y = Z$ *in the complex plane. The inverse* $r = r(y)$ *of the solution has representation* (2.44), (2.47) *taking form* (2.48) *in a neighborhood of* $y = 0$.

The convergence disc for the series on the right-hand side of (2.48) obviously does not cover the branch point $y = Z$ of analytic (with respect to y) function (2.45), which corresponds to the M-sheeted branch point $\tilde{y} = \mathcal{H}_e^{\alpha}$ of $\Theta(\tilde{y})$. To eliminate this singular point, we introduce, first, a variable $\mathcal{Y} \in [0,1]$ by the formulas

$$\tilde{y} =: \mathcal{H}_e^{\alpha}\left(1 - (1-\mathcal{Y})^M\right), \quad \mathcal{Y} = 1 - \left(1 - \frac{\tilde{y}}{\mathcal{H}_e^{\alpha}}\right)^{1/M} = 1 - \left(1 - (y/Z)^{\alpha/\beta}\right)^{1/M} \tag{2.49}$$

and, second, an analytic function on the unit interval of the form

$$\epsilon(\mathcal{Y}) := \Theta(\tilde{y}(\mathcal{Y})), \quad \frac{d\epsilon}{d\mathcal{Y}} > 0, \quad \mathcal{Y} \in [0,1], \tag{2.50}$$

which bijectively maps the interval $\mathcal{Y} \in [0,1]$ onto the parameter variation interval $t \in [0,1]$. Then inversion formula (2.45), in view of (2.49) and (2.50), can be written as follows:

$$t = \epsilon(\mathcal{Y}(y)). \tag{2.51}$$

Note that, due to (2.46) and (2.50), the expansion of $\epsilon(\mathcal{Y})$ in a neighborhood of $\mathcal{Y} = 0$ has the form

$$\epsilon(\mathcal{Y}) =: \sum_{n=1}^{\infty}\epsilon_n\mathcal{Y}^n = M\mathcal{H}_e^{\alpha}\mathcal{Y} - \left(\frac{M(M-1)}{2}\mathcal{H}_e^{\alpha} + \alpha M^2 H_1\mathcal{H}_e^{2\alpha}\right)\mathcal{Y}^2 + \cdots. \tag{2.52}$$

Upon substituting (2.50) into (2.47), we obtain the dependence of r on y in the form

$$r^{1/M} = \frac{f_0^{1/\tilde{N}}}{y^{\sigma/\tilde{N}}}(1-\epsilon(\mathcal{Y})), \quad y \in (0, Z], \quad \mathcal{Y} = \mathcal{Y}(y) \in (0,1]. \tag{2.53}$$

We raise both sides of (2.54) to the power M and substitute expansion (2.52); upon expanding brackets, we derive the following representation in a neighborhood of $y = 0$, which coincides with (1.22), for the inverse of the solution:

$$r(y) = \frac{f_0^K}{y^{1/\beta}}\left(1 - \sum_{n=1}^{\infty}\epsilon_n \mathcal{Y}^n\right)^M =: \frac{f_0^K}{y^{1/\beta}}\sum_{n=0}^{\infty} A_n' \mathcal{Y}^n, \quad A_0' = 1, \quad A_1' = -M^2\mathcal{K}_e^{\alpha}. \tag{2.54}$$

Thus, we have deduced the following theorem.

Theorem 4. *Under the assumptions of Theorem* 1, *the parameter* $t \in (0,1]$ *can be expressed in terms of* y *in form* (2.51), (2.49), *where* $\epsilon(\mathcal{Y})$ *is an analytic function on the closed interval* $\mathcal{Y} \in [0,1]$. *The inverse* $r = r(y)$ *of the solution* $y(r)$ *has representation* (2.53), *which takes form* (2.54) *in a neighborhood of* $y = 0$.

2.2. Solution of the Problem on the Interval

We derive the solution of problem (1.5)–(1.7), (1.17) with $Z, R \in (0, +\infty)$ under the assumption that the corresponding value (see Proposition 2) of the parameter $\mu \in (0,1)$ is known.

Theorem 3 in [47] asserts that the solution $\psi = \psi_\mu(\rho)$ of problem (1.26)–(1.29), (1.31) with a given μ admits the parametric representation

$$\psi = \mu(1-u)^{\tilde{N}/\sigma}(\tilde{N}u+1)^{1/\sigma}, \quad \rho = M\ln(1-u) + S(u), \quad u \in (u_1, 1], \quad u_1 := -\frac{1}{\tilde{N}}, \tag{2.55}$$

where $S(u)$ is an analytic function on the interval $u \in (u_1, 1]$ and can be expressed in the form

$$S(u) = \int^{u} s(u)du, \quad s(u) = M\frac{(\tilde{N}u+1)^{1/\sigma-1} + (1-u)^{M-1}\mathcal{P}(u)}{(\tilde{N}u+1)^{1/\sigma} + (1-u)^M\mathcal{P}(u)} \tag{2.56}$$

in terms of the solution $\mathcal{P}(u)$ of the Cauchy problem

$$\frac{d\mathcal{P}}{du} = M(\beta+1)\frac{(1-u)^{M-1}\mathcal{P}^2(u) + (\tilde{N}u+1)^{1/\sigma-1}\mathcal{P}(u) + c(u)}{(\tilde{N}u+1)^{1/\sigma} + (1-u)^M\mathcal{P}(u)}, \quad u \in (u_1, 1], \tag{2.57}$$

$$c(u) := -(\tilde{N}+1)\mu^\sigma u(\tilde{N}u+1)^{2/\sigma}(1-u)^{\tilde{N}-M-1},$$

$$\mathcal{P}(0) = -1, \quad \frac{d\mathcal{P}}{du}(0) = M(\beta+1)\left(-1 + \sqrt{\frac{(1-\mu^\sigma)(\tilde{N}+1)}{M(\beta+1)}}\right). \tag{2.58}$$

It is also shown in [47] that $\mathcal{P}(u) < 0$ for $u \in (u_1, 1]$ and that the denominator on the right-hand side of Eq. (2.57) is nonzero for $u \neq 0$.

Note that if the inclusion

$$\frac{1}{\sigma} \in \mathbb{N} \tag{2.59}$$

holds, then Eq. (2.57) satisfies the assumption of the Cauchy theorem (see [56, Section 3]) at $u = -1/\tilde{N} = u_1$; therefore, in this case, $\mathcal{P}(u)$ is also an analytic function on the whole of the interval $u \in [u_1, 1]$, including its left-hand endpoint.

Upon substituting (2.55) into (1.27) and setting

$$\mathcal{S}(u) := \exp S(u), \tag{2.60}$$

in view of (2.7), we arrive at

$$r = U_1(1-u)^M\mathcal{S}(u), \quad U_1 = \text{const} > 0, \quad u \in (u_1, 1], \tag{2.61}$$

$$y = U_2(\tilde{N}u+1)^{1/\sigma}\mathcal{S}^{-\beta}(u), \quad U_2 = \mu f_0^{1/\sigma}U_1^{-\beta}. \tag{2.62}$$

We find the value of the constant U_1 by using (2.62) and boundary condition (1.6), that is, $y = Z$ at $u = 1$:

$$U_1 = \frac{f_0{}^K \mu^{1/\beta}}{\mathcal{S}_e}(\tilde{N}+1)^K Z^{-1/\beta}, \quad \mathcal{S}_e := \mathcal{S}(u)\big|_{u=1}, \tag{2.63}$$

where K is given by (1.35).

We calculate the derivative dy/dr as a function of the parameter u. In view of (2.7), formulas (2.56), (2.60)–(2.62) yield

$$\frac{d\ln y}{du} = \frac{\tilde{N}}{\sigma(\tilde{N}u+1)} - \beta s(u) = \frac{-\beta M(\tilde{N}+1)u(1-u)^{M-1}}{(\tilde{N}u+1)\left((\tilde{N}u+1)^{1/\sigma} + (1-u)^M \mathcal{P}(u)\right)}\mathcal{P}(u), \tag{2.64}$$

$$\frac{d\ln r}{du} = -\frac{M}{1-u} + s(u) = \frac{-M(\tilde{N}+1)u(\tilde{N}u+1)^{1/\sigma-1}}{(1-u)\left((\tilde{N}u+1)^{1/\sigma} + (1-u)^M \mathcal{P}(u)\right)}, \tag{2.65}$$

which implies the following expression for the derivative:

$$\frac{dy}{dr} = \frac{y}{r}\frac{d\ln y}{du}\left(\frac{d\ln r}{du}\right)^{-1} = U_3 \mathcal{S}^{-(\beta+1)}(u)\mathcal{P}(u) < 0, \quad U_3 = \beta\frac{U_2}{U_1}\mu\beta f_0{}^{1/\sigma} U_1{}^{-(\beta+1)}.$$

Thus, we have proved the following theorem.

Theorem 5. *The solution* $y(r)$ *of problem* (1.5)–(1.7), (1.17) *with* $Z, R \in (0,+\infty)$ *admits the parametric representation*

$$r = U_1(1-u)^M \mathcal{S}(u), \quad U_1 = \frac{f_0{}^K \mu^{1/\beta}}{\mathcal{S}_e}(\tilde{N}+1)^K Z^{-1/\beta}, \quad u \in (u_1, 1], \tag{2.66}$$

$$y = U_2(\tilde{N}u+1)^{1/\sigma}\mathcal{S}^{-\beta}(u), \quad U_2 = \frac{\mathcal{S}_e^\beta}{(\tilde{N}+1)^{1/\sigma}}Z, \tag{2.67}$$

$$\frac{dy}{dr} = U_3\mathcal{S}^{-(\beta+1)}(u)\mathcal{P}(u), \quad U_3 = \beta\frac{U_2}{U_1} = \frac{\beta\mathcal{S}_e^{\beta+1}}{\mu^{1/\beta} f_0{}^K(\tilde{N}+1)^{(\beta+1)K}} Z^{(\beta+1)/\beta}, \tag{2.68}$$

where the numbers K, M, *and* $\tilde{N}$ *are given by* (1.35), $u_1 = (-1/\tilde{N})$, $\mathcal{S}(u)$ *is an analytic function on the interval* $u \in (u_1, 1]$, $\mathcal{S}_e = \mathcal{S}(1)$, *and* $\mathcal{S}(u)$ *can be represented in terms of the solution* $\mathcal{P}(u)$ *of problem* (2.57), (2.58) *in form* (2.56), (2.60). *The value of the parameter* $\mu \in (0,1)$ *entering Eq.* (2.57) *is related to the solution* $y(r)$ *by formulas* (1.31) *and* (1.25).

If condition (2.59) *is satisfied, then* $\mathcal{P}(u)$ *and* $\mathcal{S}(u)$ *are analytic functions on the whole of the interval* $u \in [u_1, 1]$, *including its left-hand endpoint* $u = u_1$.

Formula (2.68) with $u = 1$ yields the slope of the plot of the solution $y(r)$ at the endpoint $r = 0$ in the following form similar to (2.15):

$$\frac{dy}{dr}(0) = \frac{\beta Z^{(\beta+1)/\beta}}{\mu^{1/\beta} f_0{}^K(\tilde{N}+1)^{(\beta+1)K}}\mathcal{P}_e, \quad \mathcal{P}_e := \mathcal{P}(u)\big|_{u=1}. \tag{2.69}$$

It follows from (2.64), (2.65), (2.61), and (2.62) that each of the derivatives dr/du and dy/du can be represented as the product of the factor $(1-u)^{M-1}(\tilde{N}u+1)^{1/\sigma-1}$, specifying the multiplicity of zeros at the endpoints of the parametrization interval $u \in [u_1, 1]$, and some function being nonzero everywhere on this interval.

The Taylor series expansions for $\mathcal{P}(u)$, $s(u)$, and $\mathcal{S}(u)$ at $u = 0$ and other points of the interval $u \in (u_1, 1]$ can be calculated from Eq. (2.57) using the scheme described in Section 2.1.2.

2.3. Behavior of the Solution near the Origin

We show that the solution $y(r)$ of Eq. (1.5), (1.17), $Z \in (0,+\infty)$, with condition (1.6) has an expansion of form (1.19) in a neighborhood of $r = 0$. For this purpose, we use a parametric representation of this solution with a parameter z defined by (1.37).

The second formula in (1.25), substitutions (1.33) and (1.37), and equality (2.7) yield

$$\ln r = \int^{\psi} \frac{d\psi}{p(\psi)} = \int^{\psi} \frac{d\psi}{\psi q(\psi)} = \frac{\tilde{N}}{\sigma}\int^{z} \frac{dz}{zq(z)} =: \frac{\tilde{N}}{\sigma\beta}\int^{z} \frac{dz}{z} + G(z) = M\ln z + G(z), \tag{2.70}$$

where the function $G(z)$, which, in view of (1.40), has the form

$$G(z) = M\int^{z}\left(-\frac{1}{z} + \frac{1}{z\left(1 + z^{M}\mathcal{Q}(z)\right)}\right)dz = -M\int^{z} \frac{z^{M-1}\mathcal{Q}(z)}{1 + z^{M}\mathcal{Q}(z)}dz, \tag{2.71}$$

is analytic at $z = 0$ and is defined up to an additive constant. Equalities (2.70), (1.37), and (2.7) and the first formula in (1.25) implies the required parametrization

$$r = z^{M}\mathcal{G}(z), \quad y = f_0^{\;1/\sigma}\mathcal{G}^{-\beta}(z), \quad \mathcal{G}(z) := \exp G(z) \tag{2.72}$$

in a neighborhood of $z = 0$ ($r = 0$, $y = Z$), which covers representations (2.32), (2.33) and (2.66), (2.67). Note that parametric representation (2.72) in the particular case of problem (1.2), (1.3) was deduced in [40].

Using the notation $C := \mathcal{Q}(0)$ (see Proposition 3), we calculate the initial terms of the Taylor series expansions of G, $\mathcal{G}$, $r^{1/M}$, and y in powers of z relying on (2.71) and (2.72):

$$\begin{gathered} G(z) = G_0 - Cz^{M} + G_{M+1}z^{M+1} + \ldots, \quad G_0, G_{M+1} = \text{const}, \\ \mathcal{G}(z) = \mathcal{G}_0(1 - Cz^{M} + \gamma_1 z^{M+1} + \ldots), \quad \mathcal{G}_0 = \exp G_0 > 0, \quad \gamma_1 = G_{M+1} + \delta_M^1\frac{C^2}{2}, \end{gathered} \tag{2.73}$$

$$r^{1/M}(z) = \mathcal{G}_0^{1/M} z\left(1 - \frac{C}{M}z^{M} + \frac{\gamma_1}{M}z^{M+1} + \ldots\right), \tag{2.74}$$

$$y(z) = f_0^{\;1/\sigma}\mathcal{G}_0^{-\beta}(1 + \beta Cz^{M} + \gamma_2 z^{M+1} + \ldots), \quad \gamma_2 = -\beta\gamma_1 + \delta_M^1\frac{\beta(\beta+1)}{2}C^2, \tag{2.75}$$

where the Kronecker delta δ_M^1 is equal to one at $M = 1$ and zero otherwise. Due to Proposition 3, coefficients of the series inside brackets on the right-hand side of (2.73)–(2.75) can be rationally expressed in terms of β, M, $\tilde{N}$, and C. Using equality (2.75) and condition (1.6), we arrive at

$$f_0^{\;1/\sigma}\mathcal{G}_0^{-\beta} = Z, \quad \mathcal{G}_0 = f_0^{\;K}Z^{-1/\beta}. \tag{2.76}$$

By expressing z in terms of r from (2.74), we derive the following expansions in a neighborhood of $r = 0$:

$$z = \left(\frac{r}{\mathcal{G}_0}\right)^{1/M} + \frac{C}{M}\left(\frac{r}{\mathcal{G}_0}\right)^{1+(1/M)} + \gamma_3\left(\frac{r}{\mathcal{G}_0}\right)^{1+(2/M)} + \ldots, \quad \gamma_3 = -\frac{\gamma_1}{M} + \delta_M^1\frac{M+1}{M^2}C^2 \tag{2.77}$$

$$z^{M} = \frac{r}{\mathcal{G}_0} + C\left(\frac{r}{\mathcal{G}_0}\right)^{2} + M\gamma_3\left(\frac{r}{\mathcal{G}_0}\right)^{2+(1/M)} + \ldots, \tag{2.78}$$

where coefficients of the series on the right-hand sides are also rational functions of β, M, $\tilde{N}$, and C. Upon substituting (2.77) and (2.78) into (2.75), in view of (2.76), we deduce representation (1.19) in a neighborhood of $r = 0$:

$$\begin{gathered} y(r) = Z\left(1 + \frac{\beta C}{f_0^{\;K}}Z^{1/\beta}r + \gamma_4 r^{1+(1/M)} + \ldots\right) =: \sum_{n=0}^{\infty} b_n r^{n/M}, \\ \gamma_4 = \frac{\gamma_2}{\mathcal{G}_0^{1+1/M}} + \delta_M^1\frac{\beta C^2}{\mathcal{G}_0^2}, \quad b_0 = Z, \quad b_1 = \ldots = b_{M-1} = 0, \quad b_M = \frac{\beta C}{f_0^{\;K}}Z^{1+(1/\beta)}; \end{gathered} \tag{2.79}$$

according to Proposition 3, a solution $y(r)$ of form (2.79) corresponds to each $C \in \mathbb{R}$.

By the Carathéodory theorem (see [57, Ch. 2, Section 1]), a solution of the singular Cauchy problem for Eq. (1.5) with condition (1.6) and a prescribed derivative at $r = 0$ exists and is unique. We deduce the following improvement of this result.

Theorem 6. *For any* $b \in \mathbb{R}$, the Cauchy problem *for Eq.* (1.5), (1.17) *with conditions* (1.6) *and* $dy/dr(0) = b$ *is uniquely solvable on some interval* $[0, \varepsilon]$, $\varepsilon > 0$. *Its solution* $y(r)$ *can be represented in a neighborhood of* $r = 0$ *by convergent series* (2.79), *where* $b_M = b$.

Coefficients b_n of expansion (2.79) with a given $b_M = b$ can be found using the method of undetermined coefficients by substituting it into Eq. (1.5). In addition, due to (2.76) and the above-indicated properties of coefficients of expansions (2.77) and (2.78), for each $n \geq M$, the quantity $b_n f_0^{\,n/\tilde{N}}/Z^{1+(\sigma n/\tilde{N})}$ can be rationally expressed in terms of β, M, $\tilde{N}$, and $C = b_M f_0^{\,K}/(\beta Z^{1+(1/\beta)})$.

3. THOMAS–FERMI PROBLEM

The exponent $\nu = -1/2$ in the Thomas–Fermi equation (1.2) satisfies rationality condition (1.17); therefore, Theorems 1–6 proved in Section 2 are applicable to problem (1.2), (1.3). The numerical parameters introduced above (in particular, (1.9), (1.15)–(1.17), (1.36)) have the following values:

$$\nu = -\frac{1}{2}, \quad \sigma = \frac{1}{2}, \quad M = 2, \quad \tilde{N} = 3, \quad K = \frac{2}{3}, \quad \alpha = \frac{7 - \sqrt{73}}{2}, \quad \beta = 3, \quad \omega_0 = -7, \quad f_0 = 12.$$

3.1. Solution of the Thomas–Fermi Problem on the Half-Line

Representation (2.32)–(2.34) of the solution $\Psi(r)$ of problem (1.2), (1.3) with $R = +\infty$ has the form

$$\begin{gathered} r = T_1(1-t)^2 t^{1/\alpha}\mathcal{H}(t), \quad \Psi = T_2 t^{-3/\alpha}\mathcal{H}^{-3}(t), \quad \frac{d\Psi}{dr} = \frac{T_3}{t^{4/\alpha}\mathcal{H}^4(t)}\mathfrak{Q}(t), \quad t \in (0,1], \\ T_1 = \frac{12^{2/3}}{\mathcal{H}_e} Z^{-1/3}, \quad T_2 = \mathcal{H}_e^3 Z, \quad T_3 = \frac{3\mathcal{H}_e^4}{12^{2/3}} Z^{4/3}, \quad \mathcal{H}_e = \mathcal{H}(t)\big|_{t=1}, \end{gathered} \tag{3.1}$$

where $\mathfrak{Q}(t)$ and $\mathcal{H}(t)$ are analytic functions on the interval $t \in [0,1]$; $\mathfrak{Q}(t)$ is a solution of problem (2.3), (2.4), that is,

$$\frac{d\mathfrak{Q}}{dt} = 8\frac{(1-t)\mathfrak{Q}^2(t) - 1}{1 + (1-t)^2\mathfrak{Q}(t)}, \quad \mathfrak{Q}(0) = \mathfrak{Q}_0 := -1, \quad \frac{d\mathfrak{Q}}{dt}(0) = \mathfrak{Q}_1 := -2(\alpha + 1), \tag{3.2}$$

and $\mathcal{H}(t)$ can be expressed in terms of $\mathfrak{Q}(t)$ by formulas (2.2) and (2.8). Note that Eq. (3.2) was derived by E. Majorana (see [40]) directly from Eq. (1.2).

The Taylor series expansions of $\mathfrak{Q}(t)$ and $\mathcal{H}(t)$ in a neighborhood of $t = 0$ can be calculated using formulas (2.17), (2.18), (2.20), (2.22) and (2.25)–(2.29), respectively, that is,

$$\begin{gathered} g_0 = 0, \quad g_1 = -2\alpha, \quad g_n = \mathfrak{Q}_n - 2\mathfrak{Q}_{n-1} + \mathfrak{Q}_{n-2}, \quad n \geq 2, \quad \mathfrak{Q}_n \frac{V_n}{2(7 - (n+1)\alpha)}, \quad n \geq 2, \\ V_n = 8\left(-\mathfrak{Q}_0\mathfrak{Q}_{n-1} + \sum_{j=1}^{n-1}\mathfrak{Q}_j(\mathfrak{Q}_{n-j} - \mathfrak{Q}_{n-j-1})\right) - \mathfrak{Q}_1(\mathfrak{Q}_{n-2} - 2\mathfrak{Q}_{n-1}) - \sum_{j=2}^{n-1} j\,\mathfrak{Q}_j g_{n-j+1}, \quad n \geq 2, \\ h_n = -\frac{1}{2\alpha}\left(-\frac{g_{n+2}}{\alpha} + 2(\mathfrak{Q}_{n+1} - \mathfrak{Q}_n) - \sum_{j=0}^{n-1} h_j g_{n+1-j}\right), \quad H_{n+1} = \frac{h_n}{n}, \quad n \geq 0; \end{gathered} \tag{3.3}$$

the radius of convergence of these series is bounded from below by quantity (2.31): $\sqrt[6]{2} - 1 \approx 0.12$. The empirical radius of the convergence disc is ≈ 1.2, that is, this disc completely covers the domain of variation of the parameter $t \in [0,1]$.

Representation (2.54) of the inverse of the solution takes the form

$$r(\Psi) = \frac{12^{2/3}}{\Psi^{1/3}}\left(1 - \sum_{n=1}^{\infty}\epsilon_n\tilde{\Psi}^n\right)^2 =: \frac{12^{2/3}}{\Psi^{1/3}}\sum_{n=0}^{\infty}A_n'\tilde{\Psi}^n, \quad \mathcal{Y} = \tilde{\Psi} := 1 - \sqrt{1 - (\Psi/Z)^{-\alpha/3}}, \tag{3.4}$$

where the series on the right-hand side of (3.4) converge even faster that the Taylor series expansions for $\mathfrak{Q}(t)$ and $\mathcal{H}(t)$ with an empirical convergence radius of ≈ 1.8 (see Table 1 and Fig. 2). Using values of the

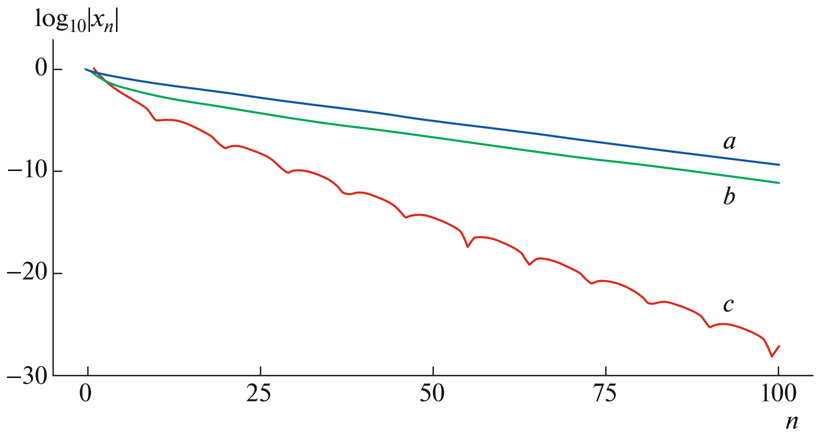

Fig. 2. Behavior of the absolute values of Taylor coefficients of the functions (*a*) $\mathcal{Q}(t)$, (*b*) $\mathcal{H}(t)$, and (*c*) $\epsilon(\tilde{\Psi})$; see (3.3) and (3.4).

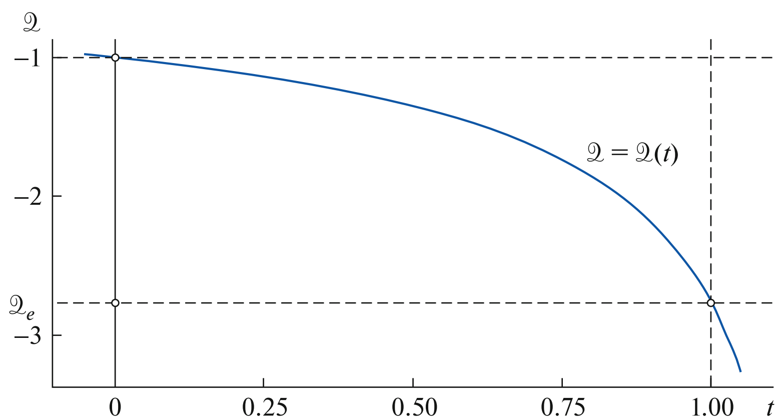

Fig. 3. Plot of the function $\mathcal{Q}(t)$; see (3.3).

coefficients ϵ_n given in Table 1, we can find the value of $\epsilon(\tilde{\Psi})$ up to 12 decimal places. Figures 3 and 4 show plots of the functions $\mathcal{Q}(t)$, $\mathcal{H}(t)$, and $\epsilon(\tilde{\Psi})$.

Representation (2.42) assumes form (1.14) with a constant A given by (2.43):

$$A = -\frac{6\mathcal{H}_e^{\alpha}}{12^{2\alpha/3}} = -13.270973848026935153531683853762148437493478662432830\ldots, \tag{3.5}$$

where, due to recurrence relations (3.3), we have

$$\mathcal{H}_e = \exp\left\{\sum_{n=1}^{\infty} H_n\right\} = 1.874501926556901049744114038434817246829720167631\ldots. \tag{3.6}$$

We now formulate the result.

Theorem 7. *The solution* $\Psi(r)$ *of problem* (1.2), (1.3) *with* $R = +\infty$ *admits parametric representation* (3.1). *Taylor coefficients for the functions* $\mathcal{H}(t)$ *and* $\mathcal{Q}(t)$ *entering it can be calculated using* (3.3) *and* (2.8). *The inverse* $r = r(\Psi)$ *of the solution admits representation* (3.4), *where the series on the right-hand side converge in a neighborhood of* $\tilde{\Psi} = \Psi = 0$. *Formula* (3.5) *is valid for the constant* A *in* (1.14).

We underline that formulas (3.5) and (3.6), based on summing an exponentially convergent numerical series each term of which can be explicitly calculated in a finite number of operations from recurrence-

Table 1. Coefficients of the Taylor series at $t = 0$ for the functions $\mathcal{Q}(t)$, $H(t) = \ln \mathcal{H}(t)$, and $\epsilon(\tilde{\Psi})$; see (3.3) and (3.4)

n	$\mathcal{Q}_n$	H_n	ϵ_n
0	−1	0	0
1	0.4559963	0.37541199	1.231293471269155
2	−0.3044551	0.11680513	−1.762572651223578E−01
3	−0.2221798	0.05301555	−3.586264513410257E−02
4	−0.1682126	0.02866072	−1.188294019140811E−02
5	−0.1298041	0.01715679	−4.527629495209355E−03
6	−0.1013002	0.01096849	−1.786511681720532E−03
7	−0.0796352	0.00733582	−6.888630288626336E−04
8	−0.0629230	0.00506758	−2.446296099146174E−04
9	−0.0499053	0.00358590	−7.102100665478879E−05
10	−0.0396962	0.00258466	−9.114850026654934E−06
11	−0.0316498	0.00189023	8.628385118260053E−06
12	−0.0252839	0.00139865	1.055443881972420E−05
13	−0.0202322	0.00104492	7.992270000062715E−06
14	−0.0162136	0.00078697	5.020985928867133E−06
15	−0.0130101	0.00059677	2.790922739565175E−06
16	−0.0104518	0.00045523	1.390873927946046E−06
17	−0.0084056	0.00034904	6.107369113157270E−07
18	−0.0067666	0.00026885	2.202119071036909E−07
19	−0.0054522	0.00020791	4.755499195027076E−08
20	−0.0043968	0.00016137	−1.546319759284382E−08
21	−0.0035485	0.00012565	−2.963705543713770E−08
22	−0.0028660	0.00009813	−2.574541382040214E−08
23	−0.0023164	0.00007684	−1.761541125892188E−08
24	−0.0018734	0.00006032	−1.043404093568663E−08
25	−0.0015161	0.00004746	−5.471632131286884E−09
26	−0.0012277	0.00003742	−2.507170177006865E−09
27	−0.0009947	0.00002956	−9.383306761822078E−10
28	−0.0008064	0.00002339	−2.107653561459858E−10
29	−0.0006540	0.00001854	6.735556420063704E−11
30	−0.0005307	0.00001472	1.344897961831818E−10
31	−0.0004309	0.00001170	1.192816857741852E−10
32	−0.0003500	0.00000932	8.286855224853180E−11
33	−0.0002844	0.00000743	4.959995317512788E−11
34	−0.0002312	0.00000593	2.612434022331377E−11
35	−0.0001880	0.00000474	1.189884390936907E−11
36	−0.0001530	0.00000379	4.309774068847392E−12
37	−0.0001245	0.00000304	7.936738883378811E−13
38	−0.0001014	0.00000243	−5.214790707757887E−13
39	−0.0000825	0.00000195	−7.998120745465573E−13
40	−0.0000673	0.00000157	−6.785731610539916E−13

type relations (3.3), differ from a similar formula (see [42, Section 2.12]) based on a parametrization of form (2.72) and requiring a numerical resolution of an indeterminacy of the form $(0 \cdot \infty)$, where the infinitely large factor is a result of numerical integration of an unboundedly increasing function.

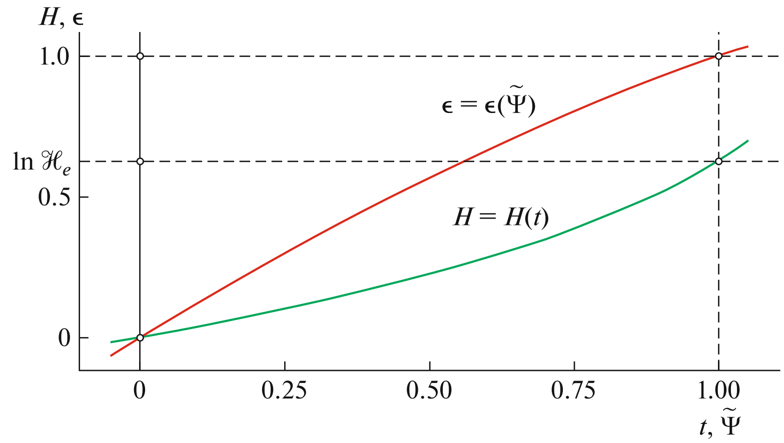

Fig. 4. Plots of the functions $H(t)$ and $\epsilon(\tilde{\Psi})$; see (3.3) and (3.4).

Note that the expression for constant (1.13) given by (2.15) with $Z = 1$, to be precise,

$$B = \frac{3\mathcal{Q}_e}{12^{2/3}} = -1.588071022611375312718684509423950109452746621674 82\ldots,$$

$$\mathcal{Q}_e = \sum_{n=0}^{\infty} \mathcal{Q}_n,$$

was derived by E. Majorana (see [40; 42, Section 2.12]).

We can calculate the solution $\Psi(r)$ and its derivative $d\Psi/dr$ at a given point $r_0 \in (0, +\infty)$ using (3.1) by finding the corresponding parameter value $t = t_0$ and substituting it into the formula $\Psi = \Psi(t_0)$. To inverse the function $r = r(t)$ by the Newton method, we should take into account that, due to (2.13), this function has a multiple zero of order $M = 2$ at $t = 1$ and its derivative is nonzero everywhere on the interval $t \in [0,1]$ except for this point. Thus, the efficiency of the Newton method for the inversion problem is guaranteed not for the very function $r(t)$ but for $\sqrt{r(t)}$ (or for $r^{1/M}(t)$ in the general case of representation (2.32)); the initial approximation for t_0 can be arbitrarily chosen on $[0,1]$.

Taking the approximation $\epsilon(\tilde{\Psi}) \approx \tilde{\Psi}$ in (3.4), we arrive at (1.23). By approximating $\epsilon(\tilde{\Psi})$, $\mathcal{Q}(t)$, and $\mathcal{H}(t)$ using some method, we can derive other efficient formulas from representations (3.1) and (3.4) to approximately solve the problem in an explicit analytic form.

3.2. Solution of the Thomas–Fermi Problem on the Interval

Representation (2.66)–(2.68) of the solution $\Psi(r)$ of problem (1.2), (1.3) with $Z, R \in (0, +\infty)$ has the form

$$r = U_1(1-u)^2\mathcal{S}(u), \quad \Psi = U_2(3u+1)^2\mathcal{S}^{-3}(u), \quad \frac{d\Psi}{dr} = U_3\mathcal{S}^{-4}(u)\mathcal{P}(u), \quad u \in (u_1, 1],$$
$$U_1 = \frac{4(36\mu)^{1/3}}{\mathcal{S}_e}Z^{-1/3}, \quad U_2 = \frac{\mathcal{S}_e^3}{16}Z, \quad U_3 = \frac{3\mathcal{S}_e^4}{64(36\mu)^{1/3}}Z^{-4/3}, \quad \mathcal{S}_e = \mathcal{S}(1), \quad u_1 = -\frac{1}{3}, \tag{3.7}$$

where $\mathcal{P}(u)$ is a solution of problem (2.57), (2.58), that is,

$$\frac{d\mathcal{P}}{du} = 8\frac{(1-u)\mathcal{P}^2(u) + (3u+1)\mathcal{P}(u) - 4\sqrt{\mu}\,u(3u+1)^4}{(3u+1)^2 + (1-u)^2\mathcal{P}(u)}, \quad u \in (u_1, 1],$$
$$\mathcal{P}(0) = -1, \quad \frac{d\mathcal{P}}{du}(0) = 8\left(-1 + \sqrt{\frac{1-\sqrt{\mu}}{2}}\right), \tag{3.8}$$

Table 2. Numerical characteristics (normalized by Z) of solutions of Thomas–Fermi problem (1.2), (1.3) with various values of the parameter μ: (1) derivative at zero, see (1.12) and (2.69); (2) ion size, $R = r(u_1)$ in (3.7); (3) ionization degree, see (1.4)

μ	$Z^{-4/3}\Psi'_r(0)$	$Z^{-1/3}R$	$1 - Z'/Z$
0.0001	−2.5864080	0.53	9.30E−01
0.02	−1.5938269	4.17	3.68E−01
0.1	−1.5881541	10.84	1.02E−01
0.2	−1.5880743	19.49	3.42E−02
0.3	−1.5880712	30.74	1.28E−02
0.4	B − 1.39E−08	46.65	4.81E−03
0.5	B − 8.16E−10	70.85	1.68E−03
0.6	B − 3.42E−11	111.14	5.14E−04
0.7	B − 7.67E−13	187.62	1.22E−04
0.8	B − 4.98E−15	369.34	1.79E−05
0.9	B − 1.41E−18	1082.77	7.83E−07
0.999	B − 6.59E−41	824236.00	1.91E−15
0.9999	B − 5.62E−52	21893653.21	1.02E−19
1.0	B	$+\infty$	0

and $\mathcal{S}(u)$ is an analytic function for $u \in (u_1, 1]$ that can be expressed in terms of $\mathcal{P}(u)$ in form (2.56), that is,

$$S(u) = 2\int_0^u \frac{(3u+1) + (1-u)\mathcal{P}(u)}{(3u+1)^2 + (1-u)^2\mathcal{P}(u)}du, \quad \mathcal{S}(u) = \exp S(u). \tag{3.9}$$

The numerical solution $\Psi(r)$ of problem (1.2), (1.3) with $R, Z \in (0, \infty)$ can be obtained using representation (3.7) in a fashion similar to the case $R = +\infty$ considered in Section 3.1. The disc of convergence of the Taylor series of $S(u)$ centered at $u = 0$ may not cover the whole of the parameter variation interval $u \in [-1/3, 1]$: in this case, we can construct Taylor series expansions for the functions $\mathcal{P}(u)$ and $S(u)$ at several other points of this interval using Eq. (3.8).

The value of μ corresponding to given $R, Z \in (0, +\infty)$ can be approximately obtained by interpolation using Table 2 (the calculations are based on (3.7)–(3.9), (2.69)).

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