EXACT SOLUTION OF INTEGRO-DIFFERENTIAL EQUATIONS OF DIFFUSION ALONG A GRAIN BOUNDARY

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Summary

We analyse model problems of stress-induced atomic diffusion from a point source or from the surface of a material into an infinite or semi-infinite grain boundary, respectively. The problems are formulated in terms of partial differential equations which involve singular integral operators. The self-similarity of these equations leads to singular integro-differential equations which are solved in closed form by reduction to an exceptional case of the Riemann–Hilbert boundary-value problem of the theory of analytic functions on an open contour. We also give a series representation and a full asymptotic expansion of the solution in the case of large arguments. Numerical results are reported.

1. Introduction

Stress-induced atomic diffusion along surfaces and grain boundaries in polycrystalline solids is an important problem for materials science and related disciplines. Structural materials subjected to high-temperature creep conditions often fail by the growth and coalescence of grain boundary cavities caused by stress-induced grain boundary diffusion (Chuang *et al.* (**1**), Spingarn and Nix (**2**), Pharr and Nix (**3**), Martinez and Nix (**4**, **5**)). More recently, stress-induced grain boundary diffusion has also been found (Thouless (**6**), Vinci *et al.* (**7**), Thompson and Carel (**8**)) to be an important mechanism of strain relaxation in thin film structures used in microelectronics, integrated optoelectronics, data storage technologies and micro-electro-mechanical systems.

Despite the importance of stress-induced grain boundary diffusion and related phenomena, there has been relatively limited effort in rigorous mathematical modelling of such phenomena. For example, one might contemplate the following fundamental questions. What is the growth rate of a stress-induced diffusion zone spreading from a point source along a grain boundary? How fast can atomic diffusion grow from a free surface into a semi-infinite grain boundary? What are the characteristic length scales and shapes of these diffusion processes? To the best of the authors' knowledge, such problems have been neither formulated nor solved in the literature. Here we develop a mathematical model which gives closed-form solutions to such problems.

Several mathematical methods form the background of the present work. Koiter (**9**) considered the problem of diffusion of load from a stiffener into a sheet and reduced it to a singular integro-differential equation on a semi-infinite axis. He applied the Mellin transform to the equation and solved the corresponding difference equation

$$T(s+1) + 2s \cot \pi s T(s) = 0 \tag{1.1}$$

in a strip of a complex variable using the Laplace transform and Alexliewsky's G-function. Bantsuri (**10**, **11**) constructed the solution of a difference equation whose natural generalization can be written as follows:

$$T(s+m) + R(s)H(s)T(s) = g(s), \quad \Re(s) = \varepsilon, \tag{1.2}$$

where $R(s)$, $H(s)$ and $g(s)$ are given; $R(s)$ is a rational function of order k at infinity: $R(s) = O(s^k)$, $s \to \infty$, $H(s)$ is a Hölder function bounded at infinity

$$H(s) = 1 + O(s^{-1}), \quad s \to \infty, \quad \Re(s) = \varepsilon\cdot \tag{1.3}$$

Bantsuri's method, based on a generalization of the Sokhotski–Plemelj formulae for a strip, is often called the method of canonical solutions. This method is efficient and rather straightforward either for the case $k = 0$ (the rational function $R(s)$ is bounded at infinity) or if the order k coincides with the modulus of the shift of the difference equation $k = \pm m$. Indeed, in the second case we may write

$$R(s) = \frac{\Gamma(s+m)}{\Gamma(s)} r(s), \tag{1.4}$$

where $\Gamma(s)$ is the Gamma function, $r(s) = C + O(s^{-1})$, $s \to \infty$, C is a constant. Thus, the second case is reducible to the first one.

Atkinson (**12**) considered a problem on anti-plane strain deformation of a composite plane with a crack, developed Koiter's approach for the case of the non-homogeneous equation (1.1) and found an exact solution of the problem in terms of Alexliewsky's G-function. An anti-plane problem and particular cases of a plane problem of fracture mechanics with special nonlinear forms of the shear modulus were analysed by Atkinson and Craster (**13**, **14**). To find an exact solution of the problems, they used the Wiener–Hopf method, Alexliewsky's G-function and Bantsuri's technique. In all cases they analysed, the corresponding difference equation satisfied the Bantsuri restriction: $k = 0$ or $k = \pm m$.

First-order difference equations in a strip arise in diffraction theory. The authors applied either Maliuzhenets's function (**15**), the solution of the factorization problem

$$f(s+2\beta) = \cot\left(\tfrac{1}{2}s + \tfrac{1}{4}\pi\right) f(s-2\beta) \tag{1.5}$$

(see, for example, Abrahams and Lawrie (**16**)) or the Barnes double-gamma functions (Lawrie and King (**17**)).

Čerskiĭ (**18**) studied an equation of smooth transition and reduced it to a particular case of the Carleman boundary-value problem for a strip (Carleman (**19**)). This case is equivalent to a difference equation in a strip. Čerskiĭ observed that the difference equation (1.1) for any function $R(s)$ of finite order at infinity, not necessarily a rational one, may be transformed into an exceptional case of the Riemann–Hilbert boundary-value problem for a semi-infinite axis. The theory of this case, namely the situation when the coefficient of the Riemann–Hilbert problem has a logarithmic singularity, was examined by Mel'nik (**20**). Tikhonenko (**21**) and Popov and Tikhonenko (**22**) found exact solutions of some problems of thermal conductivity and contact mechanics for a wedge. Their solutions were based on the results of Čerskiĭ and Mel'nik. Popov and Tikhonenko (**22**) established periodic properties of the solution but found neither a series representation nor an asymptotic expansion for the unknown function. It is worth pointing out that the corresponding difference equations (1.2), in the cases they considered, satisfied Bantsuri's conditions. However, the technique based on the results (**18**, **20** to **22**) is applicable and sufficient for any class of the coefficients of first-order difference equations.

The present work involves the following integro-differential equation:

$$uf'(u) = \int_0^\infty h\left(\frac{u}{v}\right) f'''(v)\frac{dv}{v}, \qquad 0 < u < \infty, \tag{1.6}$$

which may be reduced to Carleman's problem with the boundary condition (1.2) when $k \neq m$, where $m = 3$ is the shift and k is the order of the rational function (a polynomial of the second degree in our case). This situation leads to fractional singularities of the solution of the corresponding Riemann–Hilbert problem at the ends. We use Čerskiĭ idea of reduction of Carleman's problem to the Riemann–Hilbert problem and Mel'nik's formulae to construct an exact solution of the difference equation.

The structure of the present paper is as follows. We model atomic diffusion along an infinite and semi-infinite grain boundary and derive basic integro-differential equations in section 2.. A class of solutions is established in section 3.. Section 4. reduces the integro-differential equation of atomic diffusion along an infinite grain boundary to a Carleman boundary-value problem for a strip. Its solution is constructed in section 5. by reducing the Carleman problem to an exceptional case of the Riemann–Hilbert problem for an open contour. Section 6. represents a closed-form solution of the integro-differential equation. A series representation of the solution of the equation, the function $f(u)$, is found in section 7.1. The series converges for any bounded u. Section 7.2 develops a full asymptotic expansion of the solution for large u. In addition, in section 7.3, it is verified that the constructed solution really belongs to the class described a priori. Section 8. fits the formulae to the form convenient for calculations and discusses the numerical results. A closed-form solution of the problem of diffusion along a semi-infinite grain boundary is derived in section 9.. The behaviour of the Cauchy integral for different types of the density at the ends of the contour is derived in Appendix A. These results are necessary to find unknown parameters that are involved in the formula for the general solution of the Riemann–Hilbert problem. Periodic properties of the limit values of the solution of the Carleman problem are recorded in Appendix B. They are used for construction of the series representation and asymptotic expansion of the solution of the integro-differential equation.

2. Formulation of the problem and reduction to an integro-differential equation

We consider atomic diffusion from a point source or the surface of a material into an infinite or semi-infinite grain boundary, respectively, in response to an applied stress σ_0.

We begin by modelling an infinite grain boundary along a coordinate axis z with a point source at the origin (Fig. 1). The atomic diffusion causes a wedge of material to spread along the grain boundary. The opening displacement of the diffusion wedge can be modelled as a continuous array of climb edge dislocations. The normal traction at a position z in the boundary due to a climb edge dislocation of Burgers vector b at ζ is (Hirth and Lothe (**23**))

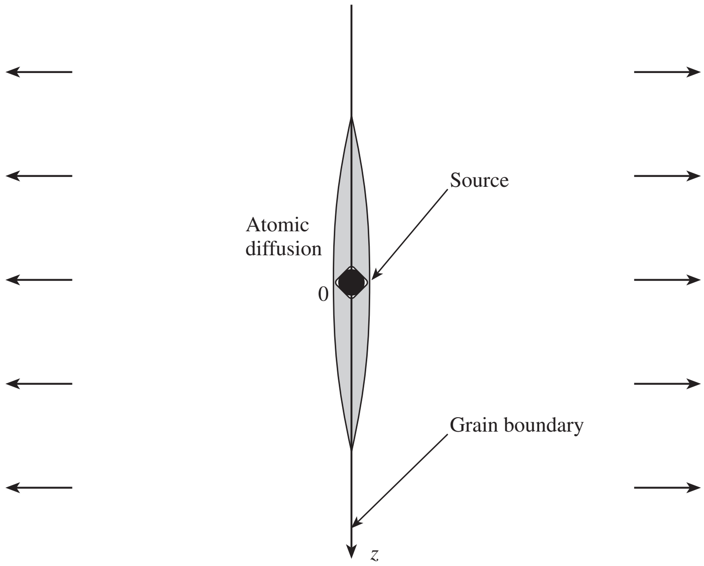

Fig. 1 Atomic diffusion along an infinite graph boundary

$$\sigma_{gb}(z,\zeta) = \frac{E^* b}{4\pi(z-\zeta)}, \tag{2.1}$$

where E^* is the plane strain elastic modulus, $E/(1-\nu^2)$. Using this solution as the Green function, the grain boundary traction σ_{gb} due to a diffusion wedge with the opening displacement function $2u(z,t)$ is

$$\sigma_{gb}(z,t) = \sigma_0 - \frac{E^*}{2\pi}\int_{-\infty}^{\infty} \frac{\partial u(\zeta,t)}{\partial \zeta}\frac{d\zeta}{z-\zeta}, \tag{2.2}$$

where σ_0 is the applied stress.

REMARK. The singular integral here and further is understood in the sense of the principal value.

We model stress-driven atomic diffusion and assume that, relative to the point source, the chemical potential at any point on the grain boundary is (Rice and Chuang (**24**))

$$\mu(z,t) = -\sigma_{gb}(z,t)\Omega\cdot \tag{2.3}$$

With this assumption, the atomic flux in the boundary per unit out-of-plane thickness is

$$j(z,t) = -\frac{\delta_{gb}D_{gb}}{kT\Omega}\frac{\partial\mu(z,t)}{\partial z} = \frac{\delta_{gb}D_{gb}}{kT}\frac{\partial\sigma_{gb}(z,t)}{\partial z}, \tag{2.4}$$

where $\sigma_{gb}(z,t)$ is the normal traction on the boundary, $\delta_{gb}D_{gb}$ is the product of the grain boundary thickness and the atomic diffusivity in the boundary, Ω is the atomic volume and kT is the product of Boltzmann's constant and temperature. Due to mass conservation, the flux divergence at any point on the boundary is related to the displacement rate at that point through

$$2\frac{\partial u(z,t)}{\partial t} = -\Omega\frac{\partial j(z,t)}{\partial z}, \tag{2.5}$$

which gives

$$\frac{\partial u(z,t)}{\partial t} = -\frac{\delta_{gb} D_{gb}\Omega}{2kT}\frac{\partial^2 \sigma_{gb}(z,t)}{\partial z^2}\cdot \tag{2.6}$$

Taking the time derivative of (2.2) and then inserting (2.6) lead to

$$\frac{\partial \sigma_{gb}(z,t)}{\partial t} = \frac{E^* D_{gb}\delta_{gb}\Omega}{4\pi kT}\int_{-\infty}^{\infty}\frac{\partial^3 \sigma_{gb}(\zeta,t)}{\partial \zeta^3}\frac{d\zeta}{z-\zeta}\cdot \tag{2.7}$$

This governing equation is supplemented by the initial condition

$$\sigma_{gb}(z,0) = \sigma_0 \tag{2.8}$$

and the boundary conditions

$$\sigma_{gb}(\infty,t) = \sigma_0, \quad \sigma_{gb}(0,t) = 0\cdot \tag{2.9}$$

The first boundary condition ensures consistency with the initial condition and the second boundary condition ensures the continuity of chemical potential near the point source.

Equation (2.7) is an unusual integro-differential diffusion equation. Assume the solution is

$$\sigma_{gb}(z,t) = \sigma_0 f(u), \tag{2.10}$$

where

$$u = z/(ct)^m\cdot \tag{2.11}$$

Substituting (2.10) and (2.11) into (2.7) and cancelling the explicit dependence on t, we find that the parameters

$$m = \tfrac{1}{3}, \qquad c = \frac{3E^*\delta_{gb}D_{gb}\Omega}{4\pi kT} \tag{2.12}$$

transform (2.7) into

$$uf'(u) = \int_{-\infty}^{\infty}\frac{f'''(v)dv}{v-u} \tag{2.13}$$

with the boundary conditions expressed as

$$f(0) = 0, \qquad f(\infty) = 1\cdot \tag{2.14}$$

A similar equation can be used to describe atomic diffusion from the surface of a material into

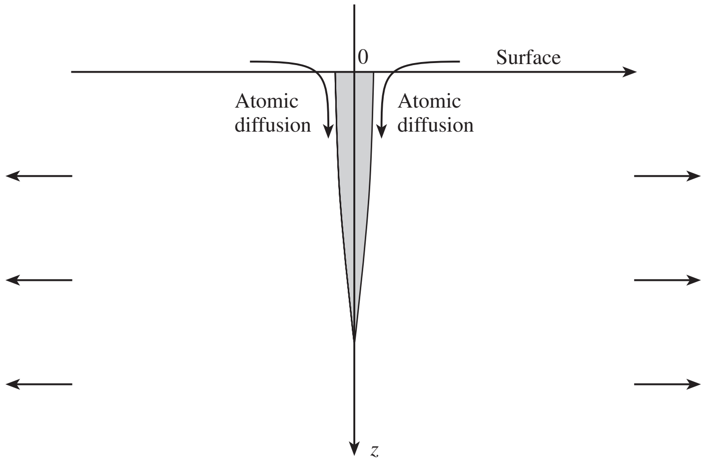

Fig. 2 Atomic diffusion along a semi-infinite grain boundary

a grain boundary in response to an applied stress σ_0 as shown in Fig. 2. In this case, the grain boundary is assumed to occupy the interval $[0, \infty)$ of the z-axis. Eshelby (**25**) has studied the elasticity problem of dislocations near a free surface. His solutions can be used as the Green function for diffusion along a semi-infinite grain boundary. According to Eshelby (**25**), the normal traction at a point z in the boundary due to a climb edge dislocation of Burgers vector b at ζ is

$$\sigma_{gb}(z,\zeta) = \frac{E^* b}{4\pi} S(z,\zeta), \quad \text{where} \quad S(z,\zeta) = \frac{1}{z-\zeta} - \frac{1}{z+\zeta} - \frac{2\zeta(z-\zeta)}{(z+\zeta)^3}\cdot \tag{2.15}$$

The grain boundary traction σ_{gb} due to a material wedge with the opening displacement function $2u(z,t)$ is

$$\sigma_{gb}(z,t) = \sigma_0 - \frac{E^*}{2\pi}\int_0^\infty S(z,\zeta)\frac{\partial u(\zeta,t)}{\partial \zeta}d\zeta, \tag{2.16}$$

where σ_0 is the applied stress. Relative to a flat, free surface, the chemical potential along the grain boundary is defined by (2.3) and similar to the infinite case, we have the grain boundary diffusion equation. This gives relation (2.6). Taking the time derivative of (2.16) and then inserting (2.6) yield

$$\frac{\partial \sigma_{gb}(z,t)}{\partial t} = \frac{E^* D_{gb}\delta_{gb}\Omega}{4\pi kT}\int_0^\infty S(z,\zeta)\frac{\partial^3 \sigma_{gb}(\zeta,t)}{\partial \zeta^3}d\zeta\cdot \tag{2.17}$$

The initial and boundary conditions are

$$\sigma_{gb}(z,0) = \sigma_0, \quad \sigma_{gb}(\infty,t) = \sigma_0, \quad \sigma_{gb}(0,t) = 0\cdot \tag{2.18}$$

The second boundary condition ensures the continuity of chemical potential near the free surface.

Similarly, we consider a solution of form

$$\sigma_{gb}(z,t) = \sigma_0 f(u), \tag{2.19}$$

where

$$u = z/(ct)^{1/3}, \qquad c = \frac{3E^*\delta_{gb}D_{gb}\Omega}{4\pi kT}\cdot \tag{2.20}$$

These transformations lead to a semi-infinite integro-differential equation

$$-uf'(u) = \int_0^\infty S(u,v)f'''(v)dv \tag{2.21}$$

with boundary conditions

$$f(0) = 0, \qquad f(\infty) = 1\cdot \tag{2.22}$$

Equation (2.21) differs from (2.13) in both the integration interval and the kernel function. The semi-infinite kernel function

$$S(u,v) = \frac{1}{u-v} - \frac{1}{u+v} - \frac{2v(u-v)}{(u+v)^3} \tag{2.23}$$

consists of three terms. The first term is identical to the Cauchy kernel in the infinite case. The second and third terms are image terms due to the presence of the free surface.

3. Class of solutions

Let us start with the problem of diffusion along an infinite grain boundary. This problem is equivalent to the following integro-differential equation:

$$uf'(u) = \int_{-\infty}^\infty \frac{f'''(v)}{v-u}dv, \qquad -\infty < u < \infty, \tag{3.1}$$

with the additional conditions

$$f(0) = 0, \qquad f(\infty) = 1\cdot \tag{3.2}$$

Due to the symmetry of the original problem, the solution of equation (3.1) is an even function and its first and third derivatives are odd:

$$f(u) = f(-u), \quad f'(u) = -f'(-u), \quad f'''(u) = -f'''(-u)\cdot \tag{3.3}$$

Since there is the factor u in the left-hand side of equation (3.1), the Fourier transformation fails in this case. To apply the Mellin transform, we take into account relations (3.3) and reduce equation (3.1) to an integro-differential equation of the Mellin convolution type on a semi-infinite interval

$$uf'(u) = 2\int_0^\infty \frac{f'''(v)}{1-(u/v)^2}\frac{dv}{v}, \qquad 0 < u < \infty\cdot \tag{3.4}$$

Let us introduce a suitable class of solutions. A function $\phi(u)$, which satisfies the Hölder condition everywhere on each finite segment $(0, C)$, except possibly the point $u = 0$ and which behaves at 0 and at infinity as

$$|\phi(u)| < Au^\alpha, \quad u \to 0; \quad |\phi(u)| < Bu^\beta, \quad u \to \infty,$$

is said to belong to the class $\mathcal{H}^{\alpha,\beta}(0,\infty)$. Here A, B, C are positive constants; α, β are real parameters. The function $f(u)$ is sought in the class $\mathcal{H}^{2-\delta,0}(0,\infty)$, where $0<\delta<1$. Then it is reasonable to assume that

$$f'(u)\in\mathcal{H}^{1-\delta,0}(0,\infty),\quad f''(u)\in\mathcal{H}^{-\delta,-1}(0,\infty),\quad f'''(u)\in\mathcal{H}^{-1-\delta,-2}(0,\infty)\cdot$$

In other words, we demand that the function $f(u)$ and its derivatives can be estimated as $u\to 0$ and $u\to\infty$ as follows:

$$|f(u)|<B_0u^{2-\delta},\quad |f^{(k)}(u)|<B_ku^{2-k-\delta}\quad (k=1,2,3),\quad u\to 0,$$
$$f(u)\sim 1,\quad |f^{(k)}(u)|<C_ku^{1-k}\quad (k=1,2,3),\quad u\to\infty\cdot \tag{3.5}$$

Here $B_m (m=0,\dots,3)$ and $C_k (k=1,2,3)$ are positive constants. It will be shown that in this class there is a unique solution of equation (3.1) with conditions (3.2).

4. Carleman boundary-value problem for a strip

Let us reduce the integro-differential equation (3.4) to a Carleman boundary-value problem of the theory of analytic functions. Due to inequalities (3.5), the Mellin transform

$$F(s)=\int_0^\infty f'''(u)u^{s-1}du \tag{4.1}$$

of the third derivative of the function $f(u)$ is analytic in the strip $1+\delta<\Re(s)<2$. We write $\Re(z)$ and $\Im(z)$ for the real and imaginary parts of a complex value z. Using integration by parts and estimations (3.5), we get

$$F(s)=(s-1)(s-2)\int_0^\infty u^{s-4}[uf'(u)]du$$
$$=-(s-1)(s-2)(s-3)\int_0^\infty u^{s-4}f(u)du,\quad 1+\delta<\Re(s)<2\cdot \tag{4.2}$$

The Mellin inversion formula yields

$$uf'(u)=\frac{1}{2\pi i}\int_\Omega\frac{F(s)}{(s-1)(s-2)}u^{3-s}ds,\quad \Omega=\{s:\Re(s)=c\} \tag{4.3}$$

uniformly with respect to $c:1+\delta<c<2$. Now let us represent the right-hand side of equation (3.4) in terms of a Mellin inverse integral. The Mellin transform of the kernel

$$\int_0^\infty\frac{2}{1-t^2}t^{s-1}dt=\pi\cot\tfrac{1}{2}\pi s$$

is analytic in the strip $0<\Re(s)<2$ (see Gradshteyn and Ryzhik (**26**, formula 3.241(3))). Due to the Mellin convolution theorem (Titchmarsh (**27**, Theorem 44)) we may write for the same contour Ω as in (4.3)

$$2\int_0^\infty\frac{f'''(v)}{1-(u/v)^2}\frac{dv}{v}=\frac{1}{2\pi i}\int_\Omega F(s)\pi\cot\tfrac{1}{2}\pi s u^{-s}ds\cdot \tag{4.4}$$

Then we introduce a new function

$$\Phi(s)=\pi\cot\tfrac{1}{2}\pi sF(s) \tag{4.5}$$

and assume that

(i) the function $\Phi(s)$ is analytically continuable into the strip $\Pi = \{-3 + c < \Re(s) < c\}$;
(ii) there exists a constant C such that

$$\int_{-\infty}^{\infty} |\Phi(x + it)|^2 dt \leqslant C \tag{4.6}$$

uniformly with respect to $x \in [-3 + c, c]$.

The last inequality provides vanishing of the function $\Phi(s)$ as $|s| \to \infty$ and $s \in \overline{\Pi}$, and gives us an opportunity to use the theory of the exceptional case of the Riemann–Hilbert boundary-value problem. It will a posteriori be shown that the function $\Phi(s)$ really satisfies all these conditions.

REMARK. The analyticity of the function $\Phi(s)$ in the strip Π and condition (4.6) mean (see Titchmarsh (**27**, Theorem 97)) that its Mellin original

$$\phi_{\mathfrak{M}}(u) = \mathfrak{M}^{-1}[\Phi(s)] = \frac{1}{2\pi i} \int_{\Omega} \Phi(s) u^{-s} ds \tag{4.7}$$

possesses the properties

$$u^c \phi_{\mathfrak{M}}(u) \in L_{2,1/u}(0, \infty), \quad u^{c-3} \phi_{\mathfrak{M}}(u) \in L_{2,1/u}(0, \infty), \tag{4.8}$$

where the weight space $L_{2,1/u}(0, \infty)$ consists of such functions $g(u)$ that

$$\int_0^{\infty} |g(u)|^2 \frac{du}{u} < \infty \cdot$$

Now we substitute relations (4.3) and (4.4) into (3.4) and exchange the function $F(s)$ for the new one $\Phi(s)$. We get

$$\frac{1}{2\pi i} \int_{\Omega} \Phi(s) u^{-s} ds = \frac{1}{2\pi i} \int_{\Omega} \frac{\Phi(s) u^{-s+3}}{\pi(s-1)(s-2)\cot\frac{1}{2}\pi s} ds, \qquad 0 < u < \infty \cdot \tag{4.9}$$

To equalize the powers of u in the latter equation, we may take into account that the function $\Phi(s)$ is analytic in the strip Π. Due to the Cauchy theorem, let us move the contour Ω in the first integral in (4.9) from the position $\Re(s) = c$ to another one: $\Omega_{-1} = \{\Re(s) = c - 3\}$. Then putting $s = s_1 - 3$ we have

$$\frac{1}{2\pi i} \int_{\Omega} \Phi(s) u^{-s} ds = \frac{1}{2\pi i} \int_{\Omega_{-1}} \Phi(s) u^{-s} ds = \frac{1}{2\pi i} \int_{\Omega} \Phi(s_1 - 3) u^{-s_1+3} ds_1 \cdot \tag{4.10}$$

Thus, equation (3.4) can be rewritten in the following equivalent form:

$$\frac{1}{2\pi i} \int_{\Omega} \left[\Phi(s-3) - \frac{\Phi(s)}{\pi(s-1)(s-2)\cot\frac{1}{2}\pi s} \right] u^{-s+3} ds = 0, \quad 0 < u < \infty \cdot \tag{4.11}$$

This means that we arrive at the following particular case of Carleman's boundary-value problem for a strip.

Find the function $\Phi(s)$ *that is analytic in the strip* $\Pi = \{-3 + c < \Re(s) < c\}$, *satisfies condition* (4.6) *and the following boundary condition:*

$$\Phi(\sigma) + K(\sigma)\Phi(\sigma - 3) = 0, \quad \sigma \in \Omega, \tag{4.12}$$

where

$$K(s) = -\pi(s-1)(s-2)\cot\tfrac{1}{2}\pi s \cdot \tag{4.13}$$

5. Exceptional case of the Riemann–Hilbert boundary-value problem

5.1 *Reduction of the Carleman problem to a Riemann–Hilbert problem*

Following the works of Čerskiĭ (**18**), Tikhonenko (**21**), Popov and Tikhonenko (**22**) we reduce the Carleman problem (4.6), (4.12) to a Riemann–Hilbert boundary-value problem for a plane with the cut along the upper semicircle. To do that we map the strip Π onto a complex plane with the cut $\gamma = \{|w| = 1, \Im(w) \geqslant 0\}$ using the 'gluing' function

$$w = i \tan\left\{\pi\left(\tfrac{1}{4} + \tfrac{1}{3}(s - c)\right)\right\}\cdot \tag{5.1}$$

The contour Ω of the s-plane is mapped onto the left-hand side ($|w| = 1 - 0$) of the contour γ of the w-plane. The right-hand side ($|w| = 1 + 0$) of the contour γ corresponds to the contour $\Omega_{-1} = \{\Re(s) = c - 3\}$ of the s-plane. The points $s = c - i\infty$ and $s = c + i\infty$ are mapped onto the points $w = 1$ and $w = -1$, respectively. Therefore, when the point s moves along Ω from the point $c - i\infty$ to $c + i\infty$, the corresponding point w moves along the contour γ in the positive direction from the starting point $a = 1$ to the terminal point $a = -1$. Then we introduce a new function

$$\varphi(w) = \frac{1}{1 + w}\left(i\frac{1 - w}{1 + w}\right)^{-1/2}\Phi(s), \tag{5.2}$$

where

$$s = c + \frac{3i}{2\pi}\log\left(i\frac{1 - w}{1 + w}\right)\cdot \tag{5.3}$$

The functions $\zeta_1(w) = \log\{i(1 - w)(1 + w)^{-1}\}$ and $\zeta_2(w) = \{i(1 - w)(1 + w)^{-1}\}^{1/2}$ are defined and analytic in the w-plane with the cut γ. Moreover, on the lower (positive) side of the contour γ, the logarithmic function $\zeta_1(\eta)$ is real and the function $\zeta_2(\eta)$ is positive. Thus, the limit values of the function $\varphi(w)$ as $w \to \eta \in \gamma^{\pm}$ are

$$\begin{aligned}(1 + \eta)\varphi^{+}(\eta) &= \exp\left\{-\tfrac{1}{3}\pi i(c - \sigma)\right\}\Phi(\sigma),\\ (1 + \eta)\varphi^{-}(\eta) &= -\exp\left\{-\tfrac{1}{3}\pi i(c - \sigma)\right\}\Phi(\sigma - 3), \quad \eta \in \gamma, \quad \sigma \in \Omega\cdot\end{aligned} \tag{5.4}$$

Here $\gamma^{+} = \{|w| = 1 - 0, \Im(w) > 0\}$, $\gamma^{-} = \{|w| = 1 + 0, \Im(w) > 0\}$. Inequality (4.6), formulated for the limit values of the function $\varphi(\zeta)$, yields

$$\left|\int_{\gamma} |\varphi^{\pm}(\eta)|^2 d\eta\right| \leqslant \text{ const}, \tag{5.5}$$

that is, $\varphi^{\pm}(\eta) \in L_2(\gamma)$. The new unknown function $\varphi(w)$ behaves at infinity as $C_0 w^{-1}$, $C_0 = \text{const}$. This follows from the definition (5.2). Due to the Čerskiĭ theorem (Čerskiĭ (**18**)), the function $\Phi(s)$ satisfies the conditions (i), (ii) if and only if the function $\varphi(w)$ can be represented as a Cauchy integral

$$\varphi(w) = \frac{1}{2\pi i}\int_{\gamma}\frac{\Sigma(\eta)}{\eta - w}d\eta, \tag{5.6}$$

where $\Sigma(\eta) \in L_2(\gamma)$. Thus, the Carleman problem (4.6) and (4.12) is equivalent to the following exceptional case of the Riemann–Hilbert boundary-value problem.

Find the function $\varphi(w)$ analytic in the w-plane with the cut γ, subject to the boundary condition

$$\varphi^+(\eta) = G(\eta)\varphi^-(\eta), \quad \eta \in \gamma, \tag{5.7}$$

where

$$G(\eta) = -\pi\left[c + \frac{3i}{2\pi}\log\left(i\frac{1-\eta}{1+\eta}\right) - 1\right]\left[c + \frac{3i}{2\pi}\ln\left(i\frac{1-\eta}{1+\eta}\right) - 2\right] \times \cot\left\{\frac{\pi}{2}\left[c + \frac{3i}{2\pi}\log\left(i\frac{1-\eta}{1+\eta}\right)\right]\right\}. \tag{5.8}$$

The function $\varphi(w)$ vanishes at infinity as w^{-1}, is representable by a Cauchy integral and its limit values $\varphi^{\pm}(\eta)$ belong to the class $L_2(\gamma)$.

Here and later we fix the branches of the logarithmic functions $\log(\eta - 1)$ and $\log(\eta + 1)$ by stipulating the inequalities

$$0 < \arg(\eta + 1) < \pi, \quad 0 < \arg(\eta - 1) < \pi, \quad \eta \in \gamma\cdot \tag{5.9}$$

The coefficient $G(\eta)$ of the problem (5.7) grows at the ends $\eta = 1$ and $\eta = -1$ of the contour γ as $\log^2(\eta - 1)$ and $\log^2(\eta + 1)$, respectively.

Mel'nik (**20**) analysed the Riemann–Hilbert problem

$$\varphi^+(t) = G(t)\varphi^-(t), \qquad t \in L \tag{5.10}$$

on the contour L that consists of a union of n simple, smooth, non-intersecting curves $a_k b_k$. The coefficient of the problem $G(t)$ is proposed to be a Hölder function on each closed portion of the curves $a_k b_k$ except at the ends. Near the ends, the function $G(t)$ admits the representation

$$G(t) = G^*(t)\ln^{r_k}(t - c_k), \quad t \to c_k, \quad c_k = a_k, b_k,$$

where r_k are real and the function $G^*(t)$ satisfies the Hölder condition on each closed curve $a_k b_k$.

In the case of the problem (5.7), the coefficient $G(\eta)$ can be represented in a neighbourhood of the points $a_{\mp} = \pm 1$ as follows:

$$G(\eta) = G_{\mp}(\eta)\log^2(\eta - a_{\mp}), \qquad \eta \to a\mp, \qquad \eta \in \gamma, \tag{5.11}$$

where

$$G_{\mp}(\eta) = G_{\mp}(a_{\mp}) + \frac{d_{\mp}}{\log(\eta - a_{\mp})} + O\left(\frac{1}{|\log(\eta - a_{\mp})|^2}\right), \quad n \to a_{\mp}, \tag{5.12}$$

$$G_{\mp}(a_{\mp}) = \pm\frac{9i}{4\pi}, \quad d_- = 3c - \frac{9}{4} - \frac{9i}{2\pi}\log 2, \quad d_+ = 3c - \frac{27}{4} + \frac{9i}{2\pi}\log 2\cdot \tag{5.13}$$

Here we took into account the formulae

$$\Im[\log(\eta - 1) - \log(\eta + 1) - \tfrac{1}{2}i\pi] = 0, \quad \eta \in \gamma,$$
$$\cot\left\{\frac{\pi}{2}\left[c + \frac{3i}{2\pi}\log\left(i\frac{1-\eta}{1+\eta}\right)\right]\right\} \to \pm i, \qquad n \to \pm 1, \qquad \eta \in \gamma\cdot \tag{5.14}$$

Thus, the Hölder condition for the function $G_{\mp}(\eta)$ fails near the end $a_{\mp}$. However, in spite of this circumstance, we may apply Mel'nik's method of solution to the problem (5.7). This follows because the canonical function of this problem and, therefore, the desirable function $\varphi(w)$ keep the same form as if it were a Hölder factor in front of the $\log^2 w$ in formula (5.11). An additional logarithmic factor in front of the main power term that defines the behaviour of the function $\varphi(w)$ at the ends of the contour will appear. It will not change the picture of solvability of the problem (5.7).

5.2 *Solution of the Riemann–Hilbert problem*

The crucial step in the solution of each Riemann–Hilbert boundary-value problem for an open contour (see Muskelishvili (**28**), Gakhov (**29**)) is to determine the increment Δ of the argument of the problem coefficient $G(\eta)$ as the point η traverses the curve γ in the positive direction. For any concrete branch of the function $\arg G(\eta)$ we define Δ as follows:

$$\Delta = [\arg G(\eta)]_{\gamma}\cdot \tag{5.15}$$

Then we take into account that

$$\log\left(\frac{1-\eta}{1+\eta}i\right) \to \mp\infty, \qquad \eta \to \pm 1 \in \gamma\cdot \tag{5.16}$$

Moreover,

$$\pm\log\left(\frac{1-\eta}{1+\eta}i\right) < 0, \quad \eta \in \gamma, \quad \pm\Re(\eta) > 0\cdot \tag{5.17}$$

At the point $\eta = i$ we have

$$\log\left(\frac{1-\eta}{1+\eta}i\right) = 0\cdot \tag{5.18}$$

Let us split the function $G(\eta)$ defined by (5.8) into three factors: $G(\eta) = g_1(\eta)g_2(\eta)g_3(\eta)$, where

$$g_m(\eta) = \begin{cases} c + \dfrac{3i}{2\pi}\log\left(i\dfrac{1-\eta}{1+\eta}\right) - m, & m = 1, 2, \\ \cot\left\{\dfrac{\pi}{2}\left[c + \dfrac{3i}{2\pi}\log\left(i\dfrac{1-\eta}{1+\eta}\right)\right]\right\}, & m = 3\cdot \end{cases} \tag{5.19}$$

For each function we observe that

$$\begin{gathered} g_1(\eta) \to -i\infty, \quad g_2(\eta) \to -i\infty, \quad g_3(\eta) \to i \quad \text{as } \eta \to 1, \\ g_1(\eta) \to c-1, \quad g_2(\eta) \to c-2, \quad g_3(\eta) \to \cot\tfrac{1}{2}\pi c \quad \text{as } \eta \to i, \\ g_1(\eta) \to i\infty, \quad g_2(\eta) \to i\infty, \quad g_3(\eta) \to -i \quad \text{as } \eta \to -1\cdot \end{gathered} \tag{5.20}$$

It is also clear from the choice of the class of solutions, that is, from the definition of the parameter c, that

$$c-1 > 0, \qquad c-2 < 0, \qquad \cot\tfrac{1}{2}\pi c < 0\cdot \tag{5.21}$$

Therefore we may conclude that

$$[\arg g_1(\eta)]_\gamma = \pi, \quad [\arg g_2(\eta)]_\gamma = -\pi, \quad [\arg g_3(\eta)]_\gamma = \pi\cdot \tag{5.22}$$

Hence the desired value is found:

$$\Delta = [\arg g_1(\eta)]_\gamma + [\arg g_2(\eta)]_\gamma + [\arg g_3(\eta)]_\gamma = \pi\cdot \tag{5.23}$$

Let us introduce the Cauchy integral

$$Y(w) = \frac{1}{2\pi i}\int_\gamma \frac{\log G(\tau)}{\tau - w}d\tau, \tag{5.24}$$

where the density is any fixed branch of the function $\log G(\tau)$. Due to the Sokhotski–Plemelj formulae, the function $\exp\{Y(w)\}$ satisfies the boundary condition (5.7). Moreover, any function

$$X(w) = (w-1)^p(w+1)^q e^{Y(w)} \tag{5.25}$$

with arbitrary integers p and q is analytic in the whole w-plane, except at the points of the contour γ. Its limit values satisfy the boundary condition (5.7). It thus follows that formula (5.25) defines a family of solutions of equation (5.7) in the class of functions with at most algebraic growth at infinity. We have to choose the branch of the logarithmic function $\log G(\tau)$ and the parameters p and q in such a way that the conditions

$$\varphi(w) = O\left(\frac{1}{w}\right), \quad w \to \infty; \quad \left|\int_\gamma |\varphi^\pm(\eta)|^2 d\eta\right| \leqslant \text{const} \tag{5.26}$$

hold. On the contour γ, the function $G(\eta)$ is expressible in terms of the limit values $X^+(\eta)$, $X^-(\eta)$ of the function $X(w)$

$$G(\eta) = \frac{X^+(\eta)}{X^-(\eta)}, \qquad \eta \in \gamma\cdot \tag{5.27}$$

We substitute this formula into the boundary condition (5.7) and apply the analytical continuation principle and Liouville's theorem (see, for example, Gakhov (**29**)). The expression $[X(w)]^{-1}\varphi(w)$ is an entire function in the w-plane. The rate at which this function may grow at infinity is algebraic. Thus, the general representation of the function $\varphi(w)$ is

$$\varphi(w) = X(w)P_\kappa(w), \tag{5.28}$$

where $P_\kappa(w)$ is a polynomial of degree κ with arbitrary complex coefficients

$$P_\kappa(w) = C_0 + C_1 w + \cdots + C_\kappa w^\kappa, \qquad \kappa \geqslant 0\cdot \tag{5.29}$$

The integer κ and the coefficients $C_0, \ldots, C_\kappa$ are to be determined.

5.3 *Satisfaction of the auxiliary conditions*

Let us satisfy conditions (5.26) and find the parameters p, q, κ and choose the branch of the function $\log G(\tau)$. The solution must vanish at infinity. From (5.24), (5.25) and (5.28) we get

$$\varphi(w) = O(w^{p+q+\kappa}), \qquad w \to \infty, \tag{5.30}$$

and therefore

$$p + q + \kappa = -1\cdot \tag{5.31}$$

To satisfy condition (5.5), we have to study the singularities of the function $\varphi(w)$ at the points $w = -1$, $w = 1$. The behaviour of the Cauchy integral

$$Y(w) = \frac{1}{2\pi i}\int_\gamma \frac{\log G(\tau)}{\tau - w} d\tau \tag{5.32}$$

in a neighbourhood of the ends of the contour γ is studied in Appendix A. Therefore it is straightforward to deduce formulae describing the behaviour of the fundamental function $X(w)$ at the points $a_- = 1$ and $a_+ = -1$:

$$\exp\{Y(w)\} = (w - a_\mp)^{\Re\{\nu_\mp(a_\mp)\}} \log^{\mu_\mp}(w - a_\mp)\Xi_\mp(w), \qquad w \to \mp a, \tag{5.33}$$

where

$$\Re\{\nu_\mp(a_\mp)\} = \mp 1 \mp \frac{1}{2\pi}\Im\{\log G_\mp(\mp)\},$$
$$\mu_\mp = 1 \mp \frac{1}{2\pi}\Im\left\{\frac{d_\mp}{G_\mp(a_\mp)}\right\} = \pm\tfrac{1}{2} + \frac{2c}{3}, \tag{5.34}$$

where $\Xi_\mp(w)$ are bounded as $w \to \mp a$ and have the definite limits $\Xi_\mp(\mp a)$. To find the values of $\Re\{\nu_\mp(a_\mp)\}$, we need to fix the arguments

$$\theta_- = \arg G_-(1), \qquad \theta_+ = \arg G_+(-1)\cdot \tag{5.35}$$

Due to formulae (5.11) and (A.16), we obtain for any fixed branch of the function $\log G(\tau)$

$$\lim_{\tau\to 1} \arg G(\tau) = \arg G_-(1) + 2\arg\log(\tau - 1) = \theta_- + 2\pi\cdot \tag{5.36}$$

Similarly,

$$\arg G(-1) = \theta_+ + 2\pi\cdot \tag{5.37}$$

It is clear from (5.13) and (5.35) that

$$\theta_- = \tfrac{1}{2}\pi + 2k\pi, \qquad k = 0, \pm 1, \pm 2, \ldots\cdot \tag{5.38}$$

Definition (5.15) of the increment Δ yields

$$\arg G(-1) = \arg G(1) + \Delta, \tag{5.39}$$

and $\Delta = \pi$ (see (5.23)). From (5.36), (5.37) we obtain the link between θ_- and θ_+: $\theta_+ = \pi + \theta_1$ and therefore

$$\theta_+ = \tfrac{3}{2}\pi + 2k\pi\cdot \tag{5.40}$$

Now we may evaluate the values $\Re\{\nu_-(1)\}$, $\Re\{\nu_+(-1)\}$:

$$\Re\{\nu_-(1)\} = -1 - \frac{\theta_-}{2\pi} = -\frac{5}{4} - k, \qquad \Re\{\nu_+(-1)\} = 1 + \frac{\theta_+}{2\pi} = \frac{7}{4} + k\cdot \tag{5.41}$$

Formulae (5.33), (5.34) and (5.41) enable us to determine the desirable behaviour of the function $X(w)$ (equation 5.25) at the end points 1, -1:

$$\begin{aligned} X(w) &= 2^q (w-1)^{p-k-5/4} \log^{\mu_-}(w-1)\,\Xi_-(1), \qquad w \to 1, \\ X(w) &= (-2)^p (w+1)^{q+k+7/4} \log^{\mu_+}(w+1)\,\Xi_+(-1), \qquad w \to -1, \end{aligned} \tag{5.42}$$

and therefore $\varphi(w)$, the function defined in (5.28), behaves at the ends of the contour γ as follows:

$$\begin{aligned} \varphi(w) &= A_-(w-1)^{p-k-5/4} \log^{\mu_-}(w-1), \qquad w \to 1, \\ \varphi(w) &= A_+(w+1)^{-p-\kappa+k+3/4} \log^{\mu_+}(w+1), \qquad w \to -1, \end{aligned} \tag{5.43}$$

where A_- and A_+ are constants. Here we used relation (5.31). The behaviour of the limit values $\varphi^{\pm}(\eta)$ of the function $\varphi(w)$ can be derived similarly if we take into account the Sokhotski–Plemelj formulae and relation (A.4)

$$\begin{aligned} \varphi^{\pm}(\eta) &= A_-^{\pm}(\eta-1)^{p-k-5/4} \log^{\mu_-^{\pm}}(\eta-1), \quad \eta \to 1, \quad \eta \in \gamma, \\ \varphi^{\pm}(\eta) &= A_+^{\pm}(\eta+1)^{-p-\kappa+k+3/4} \log^{\mu_+^{\pm}}(\eta+1), \quad \eta \to -1, \quad \eta \in \gamma, \end{aligned}$$

where $A_-^{\pm}$, $A_+^{\pm}$, $\mu_-^{\pm}$, $\mu_+^{\pm}$ are constants. In order for the functions $\varphi^{\pm}(\eta)$ to be L_2-functions on the contour γ, that is, to satisfy condition (5.5), it is necessary and sufficient that

$$p - k - \tfrac{5}{4} > -\tfrac{1}{2}, \qquad -p - \kappa + k + \tfrac{3}{4} > -\tfrac{1}{2}\cdot \tag{5.44}$$

The system of inequalities (5.44) yields

$$\tfrac{3}{4} < p - k < \tfrac{5}{4} - \kappa\cdot$$

If we take into account that p, k, κ are integers and $\kappa \geqslant 0$, then we obtain immediately that $\kappa = 0$, $p - k = 1$. Now we may choose $k = -1$, $p = 0$ and therefore from (5.31) $q = -1$. This shows that the polynomial $P_\kappa(w) \equiv C_0$ and C_0 is an arbitrary constant. The solution of the Riemann–Hilbert problem (5.7), (5.26) is given by

$$\varphi(w) = C_0 X(w), \tag{5.45}$$

where

$$X(w) = (w+1)^{-1} e^{Y(w)}\cdot \tag{5.46}$$

This behaves at the points $w = 1$, $w = -1$ as follows:

$$\varphi(w) = A_-(w-1)^{-1/4}\{\log(w-1)\}^{1/2+2c/3}, \quad w \to 1,$$
$$\varphi(w) = A_+(w+1)^{-1/4}\{\log(w+1)\}^{-1/2+2c/3}, \quad w \to -1, \tag{5.47}$$

and decays at infinity as w^{-1}. The arguments θ_-, θ_+ (5.35) have been found:

$$\theta_- = -\tfrac{3}{2}\pi, \quad \theta_+ = -\tfrac{1}{2}\pi$$

and therefore from (5.36), (5.37) we get

$$\arg G(1) = \tfrac{1}{2}\pi, \qquad \arg G(-1) = \tfrac{3}{2}\pi\cdot \tag{5.48}$$

Now we may say that the branch of the logarithmic function $\log G(\tau)$ in the Cauchy integral (5.32) is chosen in the following way:

$$\tfrac{1}{2}\pi \leqslant \arg G(\tau) \leqslant \tfrac{3}{2}\pi \quad \text{as} \quad \tau \in \gamma\cdot \tag{5.49}$$

Thus, the solution of the homogeneous Riemann–Hilbert problem (5.7) is defined by formulae (5.45), (5.46), (5.32) and (5.49).

6. Solution of the integro-differential equation by quadratures

Using the inverse map (5.1), (5.3) and formula (5.2) we obtain the expression for the original function $\Phi(s)$, the solution of the Carleman problem (4.12), (4.6) through the solution of the Riemann–Hilbert problem (5.7):

$$\Phi(s) = C_0 \exp\left\{\tfrac{1}{3}\pi i(c-s)\right\} Q(s), \quad s \in \Pi,$$
$$\Phi(\sigma) = C_0 \exp\left\{\tfrac{1}{3}\pi i(c-\sigma) + \tfrac{1}{2}\log K(\sigma)\right\} Q(\sigma), \quad \sigma \in \Omega,$$
$$\Phi(\sigma-3) = -C_0 \exp\left\{\tfrac{1}{3}\pi i(c-\sigma) - \tfrac{1}{2}\log K(\sigma)\right\} Q(\sigma), \quad \sigma \in \Omega, \tag{6.1}$$

where

$$Q(s) = \exp\left\{-\frac{i+\exp\left(\frac{2}{3}\pi i(c-s)\right)}{3}\int_\Omega \frac{\log K(\sigma)d\sigma}{\left[1-\exp\left\{\frac{2}{3}\pi i(\sigma-s)\right\}\right]\left[i+\exp\left\{\frac{2}{3}\pi i(c-\sigma)\right\}\right]}\right\}. \tag{6.2}$$

The boundary condition

$$\Phi(\sigma) + K(\sigma)\Phi(\sigma-3) = 0, \qquad \sigma \in \Omega, \tag{6.3}$$

of the Carleman problem (4.12), (4.6) is satisfied. It is verified by the direct substitution of expressions (6.1) into (6.3). Solution (6.1) possesses property (4.6). This is because the corresponding function $\varphi(w)$ satisfies the inequality

$$\left|\int_\gamma |\varphi(\eta+\tau)|^2 d\eta\right| \leqslant \text{ const}$$

uniformly with respect to τ, where τ is an arbitrary point of the w-plane. This fact follows from (5.47) and (5.30), (5.31) directly. Analysis of formulae (6.1), (6.2) shows that the function $\Phi(s)$ is analytic everywhere in the strip Π.

Since we are interested in the function $f(s)$, the solution of the original integro-differential equation (3.4), let us write down the expression for the Mellin transform of the third derivative of the original function, the function $F(s)$:

$$F(s) = \frac{1}{\pi} \tan \tfrac{1}{2}\pi s \Phi(s) \tag{6.4}$$

that follows from (4.5). The function $f(s)$ is found from (4.2) by the inverse Mellin transform

$$f(u) = -\frac{1}{2\pi i} \int_{\Omega} \frac{F(s)u^{3-s}ds}{(s-1)(s-2)(s-3)} = \frac{1}{2\pi i} \int_{\Omega} \frac{\Phi(s)u^{3-s}ds}{(s-3)K(s)}. \tag{6.5}$$

Here we took into account relations (4.5) and (4.13). Thus, we have constructed the solution of the integro-differential equation in the closed form through the solution (6.1) and (6.2) of the Carleman problem. This solution possesses an arbitrary constant that will be determined in the next section.

7. Series representation and asymptotic expansion of the solution of the integro-differential equation

7.1 *Series form of the solution*

Let us transform the integral representation of the solution (6.5) into the form convenient for numerical calculations. Additionally, we have to verify conditions (3.5), (4.8) and find the constant C_0. First, we use the boundary condition (4.12) of the Carleman problem and transform integral (6.5) into the form

$$f(u) = -\frac{1}{2\pi i} \int_{\Omega} \frac{\Phi(s-3)u^{3-s}ds}{s-3}. \tag{7.1}$$

Putting $s_{-1} = s - 3$, where $s \in \Omega$ and $s_{-1} \in \Omega_{-1}$, we get

$$f(u) = -\frac{1}{2\pi i} \int_{\Omega_{-1}} \frac{\Phi_+(s)}{s} u^{-s} ds. \tag{7.2}$$

To evaluate integral (6.5), we need the relations between the limit values of the function $\Phi(s)$

$$\Phi_-(s_m) = \lim_{\epsilon \to +0} \Phi(3m + it + c - \epsilon), \quad s_m = 3m + \sigma, \tag{7.3}$$

and

$$\Phi_+(s_m) = \lim_{\epsilon \to +0} \Phi(3m + it + c + \epsilon), \quad s_m = 3m + \sigma, \tag{7.4}$$

on each contour $\Omega_m = \{s : \Re(s) = 3m + c\}$, where $m = 0, \pm 1, \pm 2, \ldots$. They are given by

$$\Phi_-(s_m) = K(s_m - 3m)\Phi_+(s_m), \quad s_m \in \Omega_m, \quad m = 0, \pm 1, \pm 2, \ldots, \tag{7.5}$$

where $K(s) = -\pi(s-1)(s-2)\cot\frac{1}{2}\pi s$. The derivation of these relations is recorded in Appendix B (see also Popov and Tikhonenko (**22**)). Formula (7.5) for $m = -1$ enables us to express the integrand in terms of the limit value $\Phi_{-1}(s)$, $s \in \Omega_{-1}$:

$$f(u) = -\frac{1}{2\pi i}\int_{\Omega_{-1}} \frac{\Phi_-(s)u^{-s}ds}{\pi s(s+1)(s+2)\tan\frac{1}{2}\pi s}\cdot \tag{7.6}$$

The function $\Phi_-(s)(s \in \Omega_{-1})$ is analytically continuable into the strip $\Pi_{-1} = \{c-6 < \Re(s) < c-3\}$, where $-5+\delta < c-6 < -4$ and $-2+\delta < c-3 < -1$ $(0 < \delta < 1)$. We integrate the integrand (7.6) round the rectangular contour $\mathcal{L}_{-1}$ consisting of the portions $|\Im(s)| \leqslant R$ of the contours Ω_{-1}, Ω_{-2} and the segments $c-6 \leqslant |\Re(s)| \leqslant c-3$ of the lines $\Im(s) = \pm R$. The only poles within the contour $\mathcal{L}_{-1}$ are $s=-2$ and $s=-4$. The point $s=-2$ is a pole of the second order and $s=-4$ is a simple pole. Due to the residue theorem, letting $R \to \infty$, we obtain

$$\begin{aligned} f(u) = &-\frac{1}{\pi^2}\left[\Phi'(-2) - \Phi(-2)\left(\log u - \frac{3}{2}\right)\right]u^2 + \frac{2}{\pi^2}\frac{\Phi(-4)}{4\cdot 3\cdot 2}u^4 \\ &-\frac{1}{2\pi i}\int_{\Omega_{-2}} \frac{\Phi_+(s)u^{-s}ds}{\pi s(s+1)(s+2)\tan\frac{1}{2}\pi s}\cdot \end{aligned} \tag{7.7}$$

Further, to pass to the next strip $\Pi_{-2} = \{c-9 < \Re(s) < c-6\}$, we use relation (7.5) for $m=-2$:

$$\Phi_+(s) = -\frac{\Phi_-(s)}{\pi(s+4)(s+5)\cot\frac{1}{2}\pi s}, \quad s \in \Omega_{-2}\cdot \tag{7.8}$$

Additionally, we take into account the periodicity of the function $Q(s)$ (see (6.2))

$$Q(s) = Q(s+3m), \quad s \in \Pi, \quad m = 0, \pm 1, \pm 2, \dots \tag{7.9}$$

and therefore from (6.1)

$$\begin{aligned} \Phi(s) = (-1)^m\Phi(s+3m), \quad \Phi'(s) = (-1)^m\Phi'(s+3m), \\ s \in \Pi, \qquad m = 0, \pm 1, \pm 2, \dots\cdot \end{aligned} \tag{7.10}$$

In particular,

$$\Phi(-4) = -\Phi(-1), \quad \Phi(-2) = -\Phi(1), \quad \Phi'(-2) = -\Phi'(1)\cdot \tag{7.11}$$

We have

$$\begin{aligned} f(u) = &-\frac{u^2}{\pi^2}[\Phi(1)(\log u - \tfrac{3}{2}) - \Phi'(1)] - \frac{2}{\pi^2}\frac{\Phi(-1)}{4!}u^4 \\ &+\frac{1}{2\pi i}\int_{\Omega_{-2}} \frac{\Phi_-(s)u^{-s}ds}{\pi^2 s(s+1)(s+2)(s+4)(s+5)}\cdot \end{aligned} \tag{7.12}$$

Then, we repeat the previous procedure. The function $\Phi_-(s)$ can be continued analytically in the next strip Π_{-2}. The only pole within the strip Π_{-2} is $s=-5$, a simple pole. Therefore

$$f(u) = \frac{u^2}{\pi^2}\left[\Phi(1)\left(-\log u + \tfrac{3}{2}\right) + \Phi'(1)\right] - \frac{2}{\pi^2}\frac{\Phi(-1)}{4!}u^4 + \frac{1}{\pi^2}\frac{2\Phi(1)}{5!}u^5 + W_3\cdot \tag{7.13}$$

Here we replaced $\Phi(-5)$ by $\Phi(1)$ and

$$W_3 = \frac{1}{2\pi i}\int_{\Omega_{-3}} \frac{\Phi_-(s)u^{-s}ds}{\pi^3 s(s+1)(s+2)(s+4)(s+5)(s+7)(s+8)\tan\frac{1}{2}\pi s} \tag{7.14}$$

due to

$$\Phi_+(s) = \frac{\Phi_-(s)}{\pi(s+7)(s+8)\tan\frac{1}{2}\pi s}, \qquad s \in \Omega_{-3}\cdot \tag{7.15}$$

In the strip Π_{-3} there are two poles, $s = -8$ and $s = -10$, of the second and first order, respectively. The residue theorem yields for the integral W_3

$$W_3 = -\frac{2}{\pi^4}\frac{u^8}{\mu_8}[\Phi(1)(-\log u + \nu_8) + \Phi'(1)] + \frac{2}{\pi^4}\frac{u^{10}}{\mu_{10}}\Phi(-1) + W_4,$$

where

$$k^{-1}\mu_k = (k-1)(k-2)(k-4)(k-5)\cdots 2 \qquad (k \neq 3m),$$
$$\nu_{6j+2} = \frac{1}{6j+2} + \left(\frac{1}{6j+1} + \frac{1}{6j}\right) + \left(\frac{1}{6j-2} + \frac{1}{6j-3}\right) + \cdots + 1 \tag{7.16}$$

and

$$W_4 = -\frac{1}{2\pi i}\int_{\Omega_{-4}} \frac{\Phi_-(s)u^{-s}ds}{\pi^4 s(s+1)(s+2)(s+4)(s+5)(s+7)(s+8)(s+10)(s+11)} \tag{7.17}$$

with a simple pole at the point $s = -11$ of the integrand in the strip Π_{-4}. Finally, this procedure leads to the following series representation of the function $f(u)$:

$$f(u) = \sum_{j=0}^{\infty} \frac{(-1)^j u^{6j+2}}{\pi^{2j+2}}\left\{\frac{2}{\mu_{6j+2}}[\Phi(1)(\nu_{6j+2} - \log u) + \Phi'(1)] - \frac{2u^2}{\mu_{6j+4}}\Phi(-1) + \frac{u^3}{\mu_{6j+5}}\Phi(1)\right\}\cdot \tag{7.18}$$

The above series is absolutely convergent for all $u : |u| < \infty$. Indeed, for example,

$$\lim_{j\to\infty}\left|\frac{u^{6j+8}\nu_{6j+8}}{\pi^{2j+4}\mu_{6j+8}}\frac{\pi^{2j+2}\mu_{6j+2}}{u^{6j+2}\nu_{6j+2}}\right| = \lim_{j\to\infty}\left|\frac{u^6}{\pi^2(6j+8)(6j+7)(6j+6)(6j+4)}\right| = 0$$

and the radius of convergence of series (7.18) equals infinity. We note that, in particular,

$$f(u) \sim -\frac{1}{\pi^2}\Phi(1)u^2\log u, \qquad u \to 0, \tag{7.19}$$

and therefore $f(0) = 0$, that is, the first condition in (3.2) has been satisfied. The derivatives of the function $f(u)$ admit the following estimations as $u \to 0$:

$$f'(u) \sim -\frac{2}{\pi^2}\Phi(1)u\log u, \qquad f''(u) \sim -\frac{2}{\pi^2}\Phi(1)\log u,$$
$$f'''(u) \sim -\frac{2}{\pi^2}\Phi(1)\frac{1}{u}, \qquad u \to 0\cdot \tag{7.20}$$

Thus, the first group of conditions (3.5) in the neighbourhood of the point $u = 0$ is satisfied. We note that, due to (7.20), the right-hand side in (3.1) is understood in the generalized sense.

7.2 *Asymptotic expansion for large u*

Let us derive an asymptotic expansion for the function $f(u)$ convenient for large u. We start with the basic integral representation

$$f(u) = -\frac{1}{2\pi i}\int_\Omega \frac{\Phi(\sigma)u^{-\sigma+3}d\sigma}{(\sigma-1)(\sigma-2)(\sigma-3)\pi\cot\frac{1}{2}\pi\sigma}\cdot \tag{7.21}$$

At first we 'jump' over the contour Ω

$$\Phi_-(s) = -\pi(s-1)(s-2)\cot\tfrac{1}{2}\pi s\Phi_+(s), \qquad s\in\Omega\cdot \tag{7.22}$$

Here we used relation (7.5) for $m = 0$. Then we transform integral (7.21) into the form

$$f(u) = \frac{1}{2\pi i}\int_\Omega \frac{\Phi_+(s)}{s-3}u^{-s+3}ds\cdot \tag{7.23}$$

The function $\Phi_+(s)$ can be continued analytically into the strip $\Pi_1 = \{c < \Re(s) < c+3\}$. We integrate the function $(s-3)^{-1}\Phi_+(s)u^{3-s}$ round the contour $\mathcal{L}_1$, that is,

$$\begin{aligned}\mathcal{L}_1 =& \{\Re(s) = c, \Im(s)\in(-R,R)\}\cup\{\Re(s)\in(c,c+3), \Im(s) = -R\}\\ &\cup\{\Re(s) = c+3, \Im(s)\in(-R,R)\}\cup\{\Re(s)\in(c,c+3), \Im(s) = R\}\cdot\end{aligned}$$

The positive directions of the contours $\mathcal{L}_1$ and Ω_1 do not coincide. The only pole in the strip Π_1 is $s = 3$. The residue theorem yields

$$f(u) = -\Phi(3) + \frac{1}{2\pi i}\int_{\Omega_1}\frac{\pi(s-4)(s-5)\tan\frac{1}{2}\pi s}{s-3}\Phi_+(s)u^{-s+3}ds\cdot \tag{7.24}$$

Here we took into account the fact that $\Phi_-(s) = K(s-3)\Phi_+(s), s\in\Omega_1$. In the next strip, $\Pi_2 = \{c+3 < \Re(s) < c+6\}$, there is a simple pole at the point $s = 7$. Therefore

$$f(u) = -\Phi(3) + \frac{3\cdot 2}{2}\Phi(7)u^{-4} - \frac{1}{2\pi i}\int_{\Omega_2}\frac{\pi^2}{s-3}(s-4)(s-5)(s-7)(s-8)\Phi_+(s)u^{-s+3}ds\cdot \tag{7.25}$$

The integrand is an analytical function in the strip Π_3. We use the first relation in (7.10) and, again, continue analytically the integrand into the next strip Π_4 where there is a simple pole $s = 13$. We get

$$\begin{aligned}f(u) =& \Phi(0) + \frac{3\cdot 2}{2}\Phi(1)u^{-4} - \frac{\pi^2}{5}9\cdot 8\cdot 6\cdot 5\cdot 3\cdot 2\Phi(13)u^{-10}\\ &-\frac{1}{2\pi i}\int_{\Omega_4}\frac{\pi^3\Phi_{(s)}}{(s-3)\cot\frac{1}{2}\pi s}(s-4)(s-5)(s-7)(s-8)(s-10)(s-11)u^{-s+3}ds\cdot\end{aligned} \tag{7.26}$$

Here we took into account that $\Phi(3) = -\Phi(0)$, $\Phi(7) = \Phi(1)$. The next pole, $s = 19$, is in the strip Π_6. Finally we may write the following expansion when u is large:

$$f(u) \sim \Phi(0) + \frac{3!}{2}\Phi(1)u^{-4} - \frac{\pi^2}{5}\frac{9!\Phi(1)u^{-10}}{7\cdot 4\cdot 1} + \frac{\pi^4}{8}\frac{15!\Phi(1)u^{-16}}{13\cdot 10\cdot 7\cdot 4\cdot 1} - \cdots, \quad u\to\infty\cdot \tag{7.27}$$

Due to the second condition in (3.2), we have $\Phi(0) = 1$ and

$$f(u) \sim 1 + \frac{\Phi(1)}{2u^4} \sum_{j=0}^{\infty} \frac{(-1)^j \mu_{6j+4}}{(3j+2)^2} u^{-6j}, \qquad u \to \infty\cdot \tag{7.28}$$

The series in the right-hand side of (7.28) diverges but it is a Poincaré asymptotic expansion for large u (see, for example, Olver (**30**)). The condition $\Phi(0) = 1$ defines the constant C_0. From (6.1) we obtain

$$C_0 = \frac{e^{-\pi i c/3}}{Q(0)}\cdot \tag{7.29}$$

7.3 *Substantiation of the solution*

Let us show that the inverse Mellin transform $\phi_{\mathfrak{M}}(u)$ of the function $\Phi(s)$ satisfies conditions

$$u^c \phi_{\mathfrak{M}}(u) \in L_{2,1/u}(0,\infty), \quad u^{c-3}\phi_{\mathfrak{M}}(u) \in L_{2,1/u}(0,\infty)\cdot \tag{7.30}$$

Due to definition (4.7) of the function $\phi_{\mathfrak{M}}(u)$, the analyticity of the function $\Phi(s)$ in the strip Π and relation (7.5), we may write

$$\begin{aligned}\phi_{\mathfrak{M}}(u) &= \frac{1}{2\pi i}\int_{\Omega} \Phi_-(s) u^{-s} ds = \frac{1}{2\pi i}\int_{\Omega_{-1}} \Phi_+(s) u^{-s} ds \\ &= \frac{1}{2\pi i}\int_{\Omega_{-1}} \frac{\Phi_-(s) u^{-s} ds}{\pi(s+1)(s+2)\tan\frac{1}{2}\pi s}\cdot\end{aligned} \tag{7.31}$$

Using the procedure of section 7.1 we obtain

$$\phi_{\mathfrak{M}}(u) = -\frac{2}{\pi^2}\Phi(1)u^2 \log u + O(u^2), \qquad u \to 0\cdot \tag{7.32}$$

The above estimation yields

$$u^c \phi_{\mathfrak{M}}(u) \in L_{2,1/u}(0,A), \qquad u^{c-3}\phi_{\mathfrak{M}}(u) \in L_{2,1/u}(0,A)\cdot \tag{7.33}$$

These inequalities are valid for any positive $A < \infty$ and for $c > 1$. On the other hand, if we continue analytically the function $\Phi(s)u^{-s}$ into the strip Π_1 we get

$$\phi_{\mathfrak{M}}(u) = -\frac{1}{2\pi i}\int_{\Omega} \pi(s-1)(s-2)\cot\tfrac{1}{2}\pi s\, \Phi_+(s) u^{-s} ds\cdot \tag{7.34}$$

In this strip, there is a simple pole at the point $s = 4$. The next pole will be in the strip Π_3 at the point $s = 10$. The residue theorem leads to the following representation for large u:

$$\phi_{\mathfrak{M}}(u) = 12\Phi(1)u^{-4} + O(u^{-10}), \qquad u \to \infty\cdot \tag{7.35}$$

It is clear that

$$u^c \phi_{\mathfrak{M}}(u) \in L_{2,1/u}(a,\infty), \qquad u^{c-3}\phi_{\mathfrak{M}}(u) \in L_{2,1/u}(a,\infty) \tag{7.36}$$

for any small positive a and $c < 4$. Therefore, from (7.33) and (7.36) we may conclude that the solution satisfies conditions (4.8).

In addition, we show that as $u \to 0$ and $u \to \infty$ the left-hand side of equation (3.1) is consistent with its right-hand side. Indeed, from (7.28) we have

$$uf'(u) = O(u^{-4}), \qquad u \to \infty\cdot \tag{7.37}$$

On the other hand,

$$\int_{-\infty}^{\infty} \frac{f'''(v)}{v-u} dv = -\frac{h_0}{u} - \frac{h_1}{u^2} - \frac{h_2}{u^3} - \frac{h_3}{u^4} - \cdots, \qquad u \to \infty, \tag{7.38}$$

where

$$h_j = \int_{-\infty}^{\infty} v^j f'''(v) dv, \qquad j = 0, 1, \ldots \cdot \tag{7.39}$$

Since $f'''(v) = -f'''(-v)$ it follows that $h_0 = h_2 = 0$. Using (4.1) and (4.5) we have

$$h_1 = 2F(2) = \frac{2}{\pi} \lim_{s \to 2} \tan \tfrac{1}{2}\pi s \Phi(s) = 0 \tag{7.40}$$

(the function $\Phi(s)$ is analytic as $s \to 2$). As far as the coefficient h_3 is concerned, it is not zero. Indeed, the function $\Phi(s)$ has a simple pole at the point $s = 4$. That follows from formula (7.22). Therefore

$$h_3 = 2F(4) = \frac{2}{\pi} \lim_{s \to 4} \tan \tfrac{1}{2}\pi s \Phi(s) \neq 0, \tag{7.41}$$

that is, $h_0 = h_1 = h_2 = 0$ and $h_3 \neq 0$. Thus, the behaviour of the integral (7.38) as $u \to \infty$ is the same as that of the function $uf'(u)$.

Let now $u \to 0$. From (7.20) we have $uf'(u) = O(u^2 \log u)$, $u \to 0$. On the other hand,

$$\lim_{u \to 0} \int_{-\infty}^{\infty} \frac{f'''(v)}{v-u} dv = 2F(0) = \frac{2}{\pi} \lim_{s \to 0} \tan \tfrac{1}{2}\pi s \Phi(s) = 0 \tag{7.42}$$

(the function $\Phi(s)$ is analytic in the strip Π). Further

$$\lim_{u \to 0} \frac{d}{du} \int_{-\infty}^{\infty} \frac{f'''(v)}{v-u} dv = 0 \tag{7.43}$$

($f'''(u)$ is an odd function) and finally

$$\lim_{u \to 0} \frac{d^2}{du^2} \int_{-\infty}^{\infty} \frac{f'''(v)}{v-u} dv = 4F(-2) = \frac{4}{\pi} \lim_{s \to -2} \tan \tfrac{1}{2}\pi s \Phi(s) = \infty \tag{7.44}$$

(the function $\Phi(s)$ has a pole of the second order at the point $s = -2$) and again, the left- and right-hand sides of equation (3.1) are in good agreement.

8. Numerical results

To find the numerical values of $f(u)$, we may use the series representation (7.18) and the asymptotic expansion (7.28) (for large u). The following values:

$$\Phi(1) = \frac{Q(1)}{e^{\pi i/3}Q(0)}, \quad \Phi(-1) = \frac{e^{\pi i/3}Q(-1)}{Q(0)}, \\ \Phi'(1) = \frac{1}{e^{\pi i/3}Q(0)}[-\tfrac{1}{3}\pi i Q(1) + Q'(1)] \tag{8.1}$$

are involved in formulae (7.18), (7.28) for the function $f(u)$. Let us calculate the derivative $Q'(s)$. We take into account the integral representation (6.2) and relation (5.1). Then the function $Q(s)$ will be described by

$$Q(s) = \exp\left\{\frac{1}{2\pi i}\int_\gamma \frac{\log G(\tau)}{\tau - w}d\tau\right\}, \quad w = i\tan\left\{\pi\left(\frac{1}{4} + \frac{s-c}{3}\right)\right\}\cdot \tag{8.2}$$

Due to

$$\frac{dw}{ds} = \frac{i\pi}{3}(1 - w^2)$$

we may obtain

$$\frac{dQ}{ds} = Q(s)Q_0(s), \quad Q_0(s) = \frac{1-w^2}{6}\int_\gamma \frac{\log G(\tau)}{(\tau - w)^2}d\tau\cdot \tag{8.3}$$

To get formulae convenient for numerical calculations, we transform the integral representations for $Q(s)$, $Q_0(s)$ in such a way. We put $\tau = e^{i\theta}$. Then

$$Q(s) = \exp\left\{\frac{1}{2\pi}\int_0^\pi \frac{\log G_0(\theta)}{e^{i\theta} - w}e^{i\theta}d\theta\right\}, \qquad w \notin \gamma, \tag{8.4}$$

where

$$G_0(\theta) = -\pi(\sigma - 1)(\sigma - 2)\cot\frac{\pi\sigma}{2}, \qquad \sigma = c + \frac{3i}{2\pi}\log\left(\tan\frac{\theta}{2}\right)\cdot \tag{8.5}$$

Due to (5.48), (5.49), the branch of the function $\log G_0(\theta)$ must be chosen in the following manner:

$$\arg G_0(0) = \tfrac{1}{2}\pi, \quad \arg G_0(\pi) = \tfrac{3}{2}\pi, \\ \tfrac{1}{2}\pi < \arg G_0(\theta) < \tfrac{3}{2}\pi, \quad 0 < \theta < \pi\cdot \tag{8.6}$$

This means that

$$\log G_0(\theta) = |\log G_0(\theta)| + i\tan^{-1}\left(\frac{\Im\{G_0(\theta)\}}{\Re\{G_0(\theta)\}}\right) + i\pi\cdot \tag{8.7}$$

The function $\log G_0(\theta)$ behaves at the ends of the segments $[0, \pi]$ as follows:

$$\log G_0(\theta) = O(\log\log\theta), \qquad \theta \to 0, \\ \log G_0(\theta) = O(\log\log(\pi - \theta)), \qquad \theta \to \pi\cdot \tag{8.8}$$

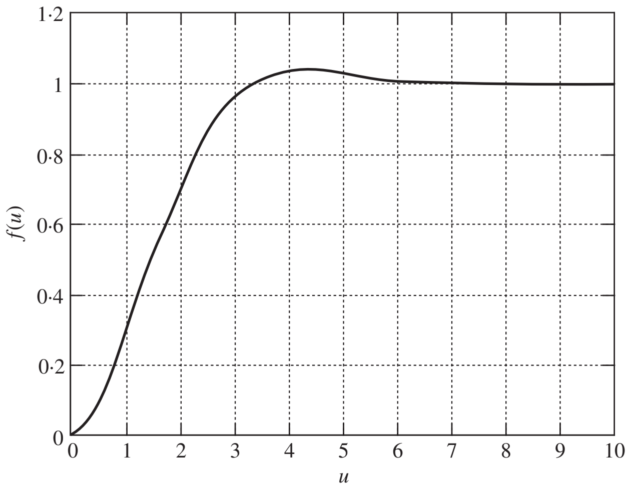

Fig. 3 The function $f(u)$

The procedure for the integral $Q_0(s)$ is the same:

$$Q_0(s) = \frac{w^2 - 1}{6i} \int_0^{\pi} \frac{\log G_0(\theta)}{(e^{i\theta} - w)^2} e^{i\theta} d\theta. \tag{8.9}$$

It is worth saying that we need the values of the functions (8.4) and (8.9) at the points $w = -1$, 0, 1 only, and the expression $e^{i\theta} - w$ in (8.4) and (8.9) does not vanish at these points. Numerical evaluation of the integrals (8.4), (8.9) yields the following values of the functions $\Phi(1)$, $\Phi(-1)$ and $\Phi'(1)$:

$$\Phi(1) = 1{\cdot}477\,258, \qquad \Phi(-1) = 1{\cdot}142\,318, \qquad \Phi'(1) = 0{\cdot}712\,287.$$

In Fig. 3 we present the graph of the function $f(u)$. It was constructed on the base of the series representation (7.18). The maximum of the function $f(u)$ occurs at the point $u = 4{\cdot}330$ and

$$\max f(u) = 1{\cdot}040\,27.$$

The asymptotic expansion (7.28) for large u is in good agreement with the series representation (7.18) for $u > 6$. Figure 4 illustrates the asymptotic expansion of function $f(u)$ for different numbers of terms of the representation (7.28). The graphs of the first, second and third derivatives of the function $f(u)$ are shown in Fig. 5.

9. Integro-differential equation of diffusion along a semi-infinite grain boundary

To solve the integro-differential equation (2.21) we modify the previous technique. The kernel $S(u, v)$ is representable in the form

$$S(u, v) = \frac{1}{v} h\left(\frac{u}{v}\right), \qquad h(t) = \frac{1}{t-1} - \frac{1}{t+1} - \frac{2(t-1)}{(t+1)^3}. \tag{9.1}$$

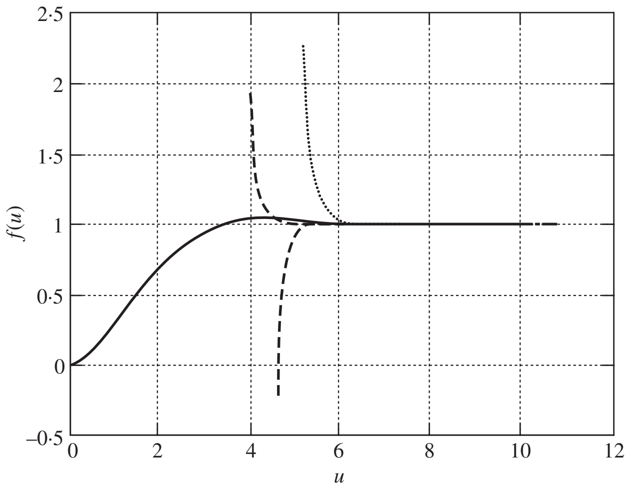

Fig. 4 The function $f(u)$: series representation (7.18) (—); asymptotic expansion (7.28) with the first four terms (- - -), five terms (–·–·), six terms (· · ·)

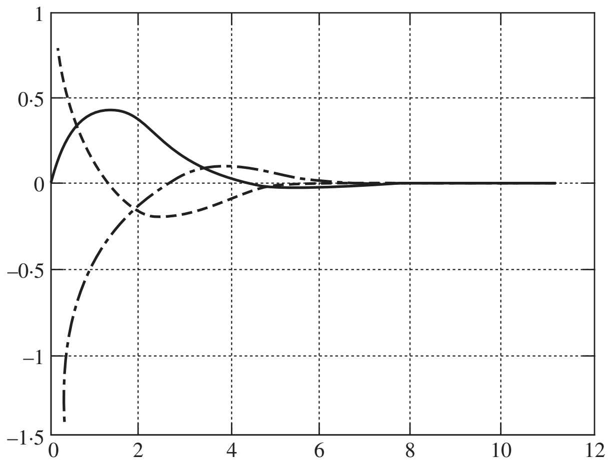

Fig. 5 Derivatives of the function $f(u)$: $f'(u)$ (—), $f''(u)$ (- - -), $f'''(u)$ (–·–·)

Due to (Gradshteyn and Ryzhik (**26**, formulae 3.222(2) and 3.194(3))), its Mellin transform is an analytic function in the strip $-1 < \Re(s) < 3$ and is given by

$$H(s) = \int_0^\infty h(t)t^{s-1}dt = -\pi \cot \pi s \left(1 + \frac{4s - 2s^2 - 1}{\cos \pi s}\right). \tag{9.2}$$

We seek the solution in the same class as before, namely, the function $f(u)$ and its derivatives are assumed to satisfy conditions (3.5). The boundary condition of the corresponding Carleman problem has the form

$$\Phi(\sigma) + d(\sigma)K(\sigma)\Phi(\sigma - 3) = 0, \quad \sigma \in \Omega, \tag{9.3}$$

where $K(\sigma)$ is the same function as in (4.13) and

$$d(s) = \cot \pi s \tan \tfrac{1}{2}\pi s \left(1 + \frac{4s - 2s^2 - 1}{\cos \pi s}\right)\cdot \tag{9.4}$$

The next step of the algorithm is to define the increment Δ introduced in (5.15). In our case, due to (5.23), we have

$$\Delta = \pi + [\arg d_0(w)]_\gamma, \tag{9.5}$$

with

$$d_0(w) = d\left(c + \frac{3i}{2\pi} \log i \frac{1 - w}{1 + w}\right)\cdot \tag{9.6}$$

Having regard to the estimations

$$\begin{aligned} &d_0(w) \sim 1, \quad \text{as} \quad w \to \pm 1, \quad w \in \gamma, \\ &d_0(i) \sim 2(2 - c) > 0 \quad \text{as} \quad c \to 2 - 0, \end{aligned} \tag{9.7}$$

we get

$$[\arg d_0(w)]_\gamma = 0\cdot \tag{9.8}$$

We note that the parameter c may be an arbitrary number: $1 + \delta < c < 2$ and $0 < \delta < 1$. Additionally, we can verify formula (9.8) numerically. Calculating the values of the $\Re\{d_0(\eta)\}$ and $\Im\{d_0(\eta)\}$ as the point η traverses the contour γ in the positive direction, we find that the increment of the argument of the function $d_0(\eta)$ is equal to zero. Therefore the solution of the Carleman problem, the complex potential $\Phi(s)$, referred to the semi-infinite grain boundary can be obtained from (6.1) and (6.2) by replacing the function $K(\sigma)$ by $d(\sigma)K(\sigma)$. The solution of the original integro-differential equation, the desirable function $f(s)$, is given by the inverse Mellin transform

$$f(u) = \frac{1}{2\pi i} \int_\Omega \frac{\Phi(s)u^{3-s}ds}{(s - 3)d(s)K(s)}\cdot \tag{9.9}$$

In this case the limit values (7.3) and (7.4) of the solution of Carleman problem (9.3) satisfy the conditions

$$\Phi_-(s_m) = d(s_m - 3m)K(s_m - 3m)\Phi_+(s_m), \quad m = 0, \pm 1, \pm 2, \ldots \cdot \tag{9.10}$$

The first step of the procedure of section 7.1 yields

$$f(u) = \frac{1}{2\pi i} \int_{\Omega_{-1}} \frac{\sin \pi s \Phi(s) u^{-s} ds}{\pi s(s + 1)(s + 2)[\cos \pi s - 4(s + 3) + 2(s + 3)^2 + 1]}\cdot \tag{9.11}$$

There are three poles of the integrand in the strip Π_{-1} : $s^{(0)} = -2$ of the second order and two complex-conjugate simple poles:

$$s^{(1)} = -4{\cdot}7396 + 1{\cdot}1190i, \qquad s^{(2)} = -4{\cdot}7396 - 1{\cdot}1190i\cdot$$

Thus, the function $f(u)$ behaves at the point $u = 0$ as follows:

$$f(u) = O(u^2 \log u), \qquad u \to 0\cdot$$

At infinity, as in the case of the infinite boundary we have $f(u) \sim 1$. The zeros of the function $d(s)$ are not periodic and therefore the final series representation and asymptotic expansion cannot be derived so straightforwardly as in the case of the infinite grain boundary. However, the function $d(s)K(s)$ is meromorphic and the procedure of section 7. may be modified for the integral (9.11).

10. Conclusion

The authors have analysed model problems of mass transport (i) from a point source into an infinite grain boundary of a material and (ii) from the surface of a material into a semi-infinite grain boundary. New unusual partial integro-differential equations of atomic diffusion have been derived. The self-similarity of the solution allows us to reduce these problems to one-dimensional singular integro-differential equations with two auxiliary conditions at zero and at infinity.

The class of functions where the solution exists and is unique has been established. The equations have been reduced to a particular case of the Carleman boundary-value problem for a strip (a first-order difference equation in a strip of a complex variable). The coefficient of the problem, the function $K(s)$, has the second order at infinity whereas the shift of the difference equation is equal to 3. Such a case, as the authors know, has been met neither in contact mechanics, nor in diffraction theory. The solution of the Carleman problem has been found by reducing to an exceptional case of the Riemann–Hilbert boundary-value problem for an open contour with coefficient that grows at the ends as a power of the logarithmic function.

The authors have constructed the exact solution of the integro-differential equations by quadratures. In the case of the infinite grain boundary, the solution, the function $f(u)$, is given in the form of a power series with infinite radius of convergence. Additionally, for large arguments, a full asymptotic expansion is derived. The final formulae involve the values of the solution of Carleman problem at two points only. The graphs for the function $f(u)$ and its first three derivatives have been represented.

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APPENDIX A

The behaviour of the Cauchy integral at the ends of the contour

Let us derive a representation of integral (5.24) in a neighbourhood of the ends of the contour γ. It is known (see Muskhelishvili (**28**)) that if γ is an open contour with ends a_- and a_+ (a_- is the starting point), and $G_*(\tau)$ is a Hölder function on the whole curve, including the ends: $G_*(\tau) \in H(\gamma)$, then

$$\frac{1}{2\pi i}\int_\gamma \frac{G^*(\tau)}{\tau - w}d\tau = \mp\frac{G^*(a_\mp)}{2\pi i}\log(w - a_\mp) + D^{(1)}_\mp(w), \quad w \to a_\mp, \tag{A.1}$$

where $D^{(1)}_\mp(w)$ are bounded in the vicinity of the points $w = a_\mp$ and tend to a definite limit as $w \to a_\mp$. The behaviour of the Cauchy integral

$$\Psi(w) = \frac{1}{2\pi i}\int_\gamma \frac{G^*(\tau)\log\log(\tau - b)}{\tau - w}d\tau \tag{A.2}$$

as $w \to b$ and b is one of the ends a_-, a_+, is described by the Mel'nik formulae (**20**)

$$\Psi(w) = \pm \frac{G^*(a_\mp)}{2\pi i}\{\log(w - a_\mp)[1 - \log\log(w - a_\mp)] \pm \pi i \log\log(w - a_\mp)\} + D_\mp^{(2)}(w), \quad w \to a_\mp, w \notin \gamma, \tag{A.3}$$

$$\Psi(\eta) = \pm \frac{G^*(a_\mp)}{2\pi i} \log(\eta - a_\mp)[1 - \log\log(\eta - a_\mp)] + D_\mp^{(3)}(\eta), \quad \eta \to a_\mp, \eta \in \gamma, \tag{A.4}$$

where the functions $D_\mp^{(2)}(w)$ are analytic in the vicinity of the points $a_\mp$, respectively, on the w-plane with the cut γ. The functions $D_\mp^{(3)}(\eta)$ are continuous at the points $\eta = a_\mp$.

The Cauchy integral with the density $1/\log(\tau - b)$ admits the representation (Zverovich (**31**))

$$\frac{1}{2\pi i}\int_\gamma \frac{d\tau}{(\tau - w)\log(\tau - a_\mp)} = \mp \frac{1}{2\pi i} \log\log(w - a_\mp) + D_\mp^{(4)}(w), \quad w \to a_\mp, \tag{A.5}$$

with the functions $D_\mp^{(4)}(w)$ that are bounded as $w \to a_\mp$. Additionally, we need the following result:

$$\frac{1}{2\pi i}\int_\gamma \frac{d\tau}{(\tau - w)\log^r(\tau - a_\mp)} = O(1), \qquad w \to a_\mp, \quad r > 1\cdot \tag{A.6}$$

It follows from the formula derived in (**31**)

$$\frac{1}{2\pi i}\int_a^\infty \frac{d\tau}{(\tau - w)\log^z(\tau - a)} = \begin{cases} \zeta\left(z, \dfrac{1}{2\pi i}\log(w - a)\right), & n > 0, \\ \zeta\left(z, 1 - \dfrac{1}{2\pi i}\log(w - a)\right), & n \leqslant 0, \end{cases} \tag{A.7}$$

that is valid for $\Re(z) > 1$. Here $\zeta(z, \alpha)$ is the generalized zeta function; the branch of the logarithmic function is fixed in such a way that $\log 1 = 2\pi n i$.

We proceed to estimate the Cauchy integral (5.32) in the vicinity of the starting point of the contour γ. Due to representations (5.11), (5.12), we have

$$\log G(\tau) = 2\log\log(\tau - 1) + \log G_-(1) + \frac{d_-}{G_-(1)\log(\tau - 1)} + O\left(\frac{1}{|\log(\tau - 1)|^2}\right) \quad \text{as} \quad \tau \to 1, \quad \tau \in \gamma\cdot \tag{A.8}$$

Using formulae (A.1), (A.3), (A.5), (A.6) we may derive

$$Y(w) = \nu_-(w)\log(w - 1) + \rho_- \log\log(w - 1) + Y_-(w), \quad w \to 1, \quad w \notin \gamma, \tag{A.9}$$

where

$$\nu_-(w) = \frac{1}{\pi i}[1 - \log\log(w - 1)] - \frac{\log G_-(1)}{2\pi i}, \qquad \rho_- = 1 + \frac{d_- i}{2\pi G_-(1)}, \tag{A.10}$$

the function $Y_-(w)$ is bounded at $w = 1$ and tends to a definite limit as $w \to 1$. As $w \to -1$ and $w \notin \gamma$ we have

$$Y(w) = \nu_+(w)\log(w + 1) + \rho_+ \log\log(w + 1) + Y_+(w), \quad w \to -1, w \notin \gamma, \tag{A.11}$$

where

$$\begin{gathered}\nu_+(w) = -\frac{1}{\pi i}[1 - \log\log(w+1)] + \frac{\log G_+(-1)}{2\pi i},\\ \rho_+ = 1 - \frac{d_+ i}{2\pi G_+(-1)},\end{gathered} \tag{A.12}$$

the function $Y_+(w)$ is bounded as $w \to -1$ and $\lim Y_+(w)$ exists as $w \to -1$. The function $\log\log(w-b)$ ($b = 1$ or $b = -1$) possesses the following properties:

$$\log\log(w-b) = \log|\log(w-b)| + i\arg Z(w) \tag{A.13}$$

with $Z(w) = \log(w-b)$. If $|w-b| < 1$ then

$$\arg Z(w) = \pi + \tan^{-1}\frac{\arg(w-b)}{\log|w-b|}\cdot \tag{A.14}$$

Assuming that $w \to b$ along any path with a finite number of circuits, one may write

$$\lim_{w\to b}\arg Z(w) = \lim_{w\to b}\Im\{\log Z(w)\} = \pi\cdot \tag{A.15}$$

This result was obtained by Mel'nik (**20**). Therefore

$$\begin{gathered}\Im\{\log\log(w-1)\} \to \pi, \quad w \to 1,\\ \Im\{\log\log(w+1)\} \to \pi, \quad w \to -1,\end{gathered} \tag{A.16}$$

and the desired behaviour of the Cauchy integral (5.24) is described by formulae (A.9) to (A.12) and (A.16).

APPENDIX B

Limit values of the solution of the Carleman problem

Analysis of the integral (6.1) shows that the function $\Phi(s)$ is analytic in each strip

$$\Pi_m = \{s : c + 3m - 3 < \Re(s) < c + 3m\} \tag{B.1}$$

and its limit values $\Phi_+(s_m)$ and $\Phi_-(s_m)$ do not coincide with each other. Directly from formulae (6.1) we get

$$\Phi_-(s_0) = \Phi(\sigma), \quad \Phi_+(s_{-1}) = \Phi(\sigma - 3), \quad \sigma \in \Omega_0 = \Omega\cdot \tag{B.2}$$

Then

$$\begin{gathered}\Phi_+(s_0) = C_0\exp\{\tfrac{1}{3}\pi i(c-\sigma)\}Q(\sigma)\exp\{-\tfrac{1}{2}\log K(\sigma)\} = -\Phi(\sigma-3),\\ \Phi_-(s_1) = C_0\exp\{\tfrac{1}{3}\pi i(c-s_1)\}\lim_{s\to s_1, s\in\Pi_1} Q(s)\cdot\end{gathered} \tag{B.3}$$

Putting in the above formula $s_1 = \sigma + 3$ we obtain

$$\Phi_-(s_1) = -C_0\exp\{\tfrac{1}{3}\pi i(c-\sigma)\}\lim_{s\to\sigma, s\in\Pi} Q(s)\cdot \tag{B.4}$$

From the Sokhotski–Plemelj formulae we have

$$\lim_{s\to\sigma, s\in\Pi} Q(s) = \exp\left\{\tfrac{1}{2}\log K(\sigma)\right\}Q(\sigma), \quad \sigma\in\Omega\cdot \tag{B.5}$$

Thus, $\Phi_-(s_1) = -\Phi(\sigma)$, $\sigma \in \Omega$. In a similar way, one may deduce that

$$\Phi_-(s_m) = (-1)^m\Phi(\sigma), \quad \Phi_+(s_m) = (-1)^{m+1}\Phi(\sigma-3), \quad m = 0, \pm1, \pm2, \ldots\cdot \tag{B.6}$$

Now we substitute formulae (B.6) into the boundary condition (4.12) and multiply by $(-1)^m$:

$$(-1)^m\Phi(\sigma) = (-1)^{m+1}\Phi(\sigma-3)K(\sigma), \quad \sigma\in\Omega\cdot \tag{B.7}$$

Then we put $s_m - 3m$ instead of σ and use relations (B.6). The limit values of the function $\Phi(s)$ on each contour Ω_m are linked by $\Phi_-(s_m) = K(s_m - 3m)\Phi_+(s_m)$, $s_m \in \Omega_m$, $m = 0, \pm1, \pm2, \ldots$.