

## ADSORPTION INTEGRAL EQUATION

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**ABSTRACT.** The relationship between the measured adsorption isotherm and unknown energy distribution function is described by so-called adsorption integral equation, a linear Fredholm integral equation of the first kind. We show that under rather general assumptions the equation can be solved in an analytical form. We also develop some methods to construct approximate solutions.

**1. Introduction.** The relationship between the measured adsorption isotherm and unknown energy distribution function is described by so-called adsorption integral equation, a linear Fredholm integral equation of the first kind

$$(1) \quad \theta(p) = \int_0^{\infty} \theta(p, E)N(E) dE,$$

where  $p$  is a pressure,  $E$  is an energy,  $\theta(p, E)$  is a local adsorption isotherm,  $\theta(p)$  is a global adsorption isotherm, and  $N(E)$  is a relative number of adsorbing centers with the energy  $E$ , see [13]. The function  $N$  is defined for nonnegative values of  $E$ , takes nonnegative values, and satisfies the condition

$$(2) \quad \int_0^{\infty} N(E) dE = 1.$$

Without proof but giving several examples, Rudzinski and Everett [13] showed that the detailed form of any theoretical isotherm is determined by the form of function  $\xi(\theta, T)$  satisfying

$$(3) \quad \ln(pK_0) = -E/K_B T + \ln \xi(\theta, T)$$

where  $E$  is the adsorption energy,  $T$  is the temperature,  $K_B$  is the Boltzmann constant, and  $K_0$  is a function of the temperature. This statement has been proved in [12]. Equation 3 means that, provided that the inverse function of  $\xi$  exists, the local isotherm  $\theta(p, E)$  has the form

$$\theta(p, E) = \Theta(K(E)p),$$

where  $K(E) = K_0 \exp(E/K_B T)$ . In the sequel we assume that  $K_0$  is a constant. Introducing the variable  $K = K(E)$ , we obtain the integral equation

$$(4) \quad \theta(p) = \int_0^\infty \Theta(Kp) \mathcal{N}(K) dK,$$

where

$$\mathcal{N}(K) = \begin{cases} 0 & K \in [0, K_0], \\ K_B T N(E(K))/K & K \in (K_0, +\infty). \end{cases}$$

Integral equation (4) can be solved applying the Mellin transform or after some change of variables it can be reduced to a convolution form and solved using the Fourier transform. However all these general methods work only under rather restrictive assumptions on the functions  $\theta$  and  $\Theta$  that are not satisfied in the problems arising in the adsorption theory. Therefore some special methods are needed.

We show that, under some natural assumptions, the local isotherm has the form

$$\Theta(Kp) = \sum_{j=1}^{\infty} Q_j \left( \frac{Kp}{1+Kp} \right)^j, \quad \text{Re}(Kp) > -\frac{s_a}{2}, \quad s_a > 0,$$

where  $K = K(E) = K_0 \exp(E/K_B T)$ ,  $T$  is a temperature,  $K_B$  is the Boltzmann constant and  $K_0$  is a constant. If  $Q_1 = 1$  and  $Q_j = 0$ ,  $j > 1$ , then we get the Langmuir local isotherm (Langmuir kernel)

$$\Theta(Kp) = \frac{Kp}{1+Kp}.$$

It is well known that in this case equation (1) can be reduced to the Stieltjes integral equation [14, 15]. In order to reduce the general integral equation to the Langmuir equation we consider the case when the kernel is a polynomial of Langmuir's kernel:

$$\Theta(Kp) = \sum_{j=1}^J Q_j \left( \frac{Kp}{1+Kp} \right)^j.$$

We show that the function

$$G(p) = \int_0^\infty \frac{K}{1+Kp} \mathcal{N}(K) dK$$

is a unique solution to the Euler differential equation

$$\frac{\theta(p)}{p} = \sum_{j=0}^{J-1} \frac{(-1)^j Q_{j+1}}{j!} p^j G^{(j)}(p)$$

satisfying the boundary conditions

$$\lim_{p \rightarrow 0} pG(p) = 0 \quad \text{and} \quad \lim_{p \rightarrow \infty} pG(p) = 1.$$

This solution to the Euler equation can be easily found. Passing to the limit when the degree  $J$  of the polynomial tends to infinity, we get the solution in the general case and therefore find the function

$$\mathcal{L}(\mathcal{N})(p) = \int_0^\infty \frac{Kp}{1 + Kp} \mathcal{N}(K) dK, \quad p > 0.$$

Thus the general case can be reduced to the Langmuir integral equation.

We develop also some methods to construct an approximate solution to the adsorption integral equation. In chemical experiments the global isotherm  $\theta$  is known only at some points  $p_l > 0$ ,  $l = 1, 2, \dots, L$ . We show that if  $L \rightarrow \infty$ , this information is enough to reconstruct the function  $\theta(p)$ ,  $p > 0$ . Solving the Euler equation one can find the function  $\mathcal{L}(\mathcal{N})(p)$ ,  $p > 0$ . Then it remains to solve the Stieltjes equation in order to find the distribution function  $\mathcal{N}$ . We reduce the reconstruction of  $\theta(p)$  and the solution of the Stieltjes equation to a problem of complex analytic continuation with prescribed bound. This problem was largely studied, see [1, 2, 5, 6, 8, 10, 11, 16], for example. The method presented in this paper is closed in spirit to the mentioned works. The main feature of our approach is the use of condition (2) to derive the bounds for the Taylor coefficient of the analytic function to be found. These bounds guarantee the method's stability with respect to small perturbations of the data. The numerical algorithms constructed on the base of this approach allow to reduce the problem under consideration to a linear-quadratic programming problem. In [3] the method has been compared with the Tikhonov regularization method in the case of the Langmuir kernel. The results of numerical experiments show that if the distribution has a relatively small  $L_2$ -norm, the both methods give close results. On the other hand,

if the distribution's  $L_2$ -norm is big, the Tikhonov regularization does not work while the algorithm based on the complex approximation with constraints gives acceptable reconstruction. This may be of importance if the distribution is composed of one or several narrow 'peaks' and has a big  $L_2$ -norm. Numerical experiments in the case of the kernel of general form can be found in [4].

The paper is organized as follows. In the second section we introduce the class of kernels used in the sequel and establish some properties of local and global isotherms. The third section contains the main inversion result for the adsorption integral equation. The fourth section is devoted to approximate methods and to the problem of complex analytic continuation.

**2. Properties of local and global isotherms.** In this section we describe the class of kernels considered in the sequel and study some properties of local and global isotherms. We consider the local isotherms with the following structure. They depend on the product  $K(E)p$ :

$$(5) \quad \theta(p, E) = \Theta(K(E)p),$$

where  $K(E) = K_0 \exp(E/K_B T)$ ,  $T$  is a temperature,  $K_B$  is the Boltzmann constant and  $K_0$  is a constant. Introducing the variable  $K = K(E)$ , from (1) and (2) we get

$$(6) \quad \theta(p) = \int_0^\infty \Theta(Kp) \mathcal{N}(K) dK$$

and

$$(7) \quad \int_0^\infty \mathcal{N}(K) dK = 1,$$

respectively, where

$$(8) \quad \mathcal{N}(K) = \begin{cases} 0 & K \in [0, K_0], \\ K_B T N(E(K))/K & K \in (K_0, +\infty). \end{cases}$$

We assume that the function  $\Theta = \Theta(s)$  satisfies the following conditions:

1. The function  $\Theta$  is monotone non-decreasing in the real positive ray:  $\Theta'(s) \geq 0$ , whenever  $s \geq 0$ .
2.  $\Theta(0) = 0$  and  $\lim_{s \rightarrow +\infty} \Theta(s) = 1$ .
3. The function  $\Theta$  is analytic in the half-plane  $\text{Re}: z > -s_a/2, s_a > 0$ .

The function  $\Theta$  satisfies the first two conditions because of physical reasons [13–15]. Condition 3 is essential for the approach presented below.

Without loss of generality  $s_a = 1$ . (The case  $s_a \neq 1$  can be reduced to this one by a change of variables.)

Consider the Möbius transformation  $q = s/(1+s)$ . It maps the semi-plane  $\text{Re}: s > -1/2$  onto the unit disk  $D = \{q \mid |q| < 1\}$ . The function  $Q(q) = \Theta(s(q))$  is analytic in  $D$  and we have

$$(9) \quad Q(q) = Q_1q + Q_2q^2 + \dots + Q_nq^n + \dots, \quad |q| < 1.$$

From this we obtain

$$(10) \quad \Theta(Kp) = \sum_{j=1}^{\infty} Q_j \left( \frac{Kp}{1+Kp} \right)^j, \quad \text{Re}(Kp) > -\frac{1}{2}.$$

Under some additional assumptions on the coefficients  $Q_j, j = 1, 2, \dots$ , one can obtain boundedness conditions for the function  $\Theta$ .

**Proposition 1.** *Assume that Condition 3 is satisfied.*

1. *If  $\sum_{j=1}^{\infty} |Q_j| < \infty$ , then the function  $\Theta$  is bounded in the half-plane  $\text{Re}: z \geq 0$ :*

$$\sup_{\{s \mid \text{Re}: s \geq 0\}} |\Theta(s)| \leq M.$$

2. *If  $\sum_{j=1}^{\infty} j|Q_j| < \infty$ , then the function  $\Theta'(s)s$  is bounded in the half-plane  $\text{Re}: z \geq 0$ :*

$$\sup_{\{s \mid \text{Re}: s \geq 0\}} |\Theta'(s)s| \leq M.$$

*Proof.* 1. Observe that

$$\left| \frac{\rho e^{i\lambda}}{1 + \rho e^{i\lambda}} \right| = \frac{\rho}{\sqrt{1 + 2\rho \cos \lambda + \rho^2}}.$$

Suppose that  $\sum_{j=1}^{\infty} |Q_j| < \infty$ . Then we have

$$|\Theta(\rho e^{i\lambda})| \leq \sum_{j=1}^{\infty} |Q_j| \left( \frac{\rho}{\sqrt{1 + 2\rho \cos \lambda + \rho^2}} \right)^j < \sum_{j=1}^{\infty} |Q_j|,$$

whenever  $\lambda \in [-\pi/2, \pi/2]$ .

2. Now suppose that  $\sum_{j=1}^{\infty} j|Q_j| < \infty$ . Then we get

$$\begin{aligned} & |\Theta'(\rho e^{i\lambda}) \rho e^{i\lambda}| \\ & \leq \sum_{j=1}^{\infty} j|Q_j| \left( \frac{\rho}{\sqrt{1 + 2\rho \cos \lambda + \rho^2}} \right)^j \left( \frac{1}{\sqrt{1 + 2\rho \cos \lambda + \rho^2}} \right) \\ & < \sum_{j=1}^{\infty} j|Q_j|, \end{aligned}$$

whenever  $\lambda \in [-\pi/2, \pi/2]$ .  $\square$

The main properties of the global isotherm  $\theta(p)$  are contained in the following proposition.

**Proposition 2.** *The function  $\theta$  has the following properties:*

1.  $\theta(p_1) \leq \theta(p_2)$ , whenever  $0 \leq p_1 \leq p_2$ ;
2.  $\lim_{p \rightarrow 0^+} \theta(p) = 0$  and  $\lim_{p \rightarrow +\infty} \theta(p) = 1$ ;
3. If the function  $\Theta$  is bounded in the half-plane  $\operatorname{Re}: z \geq 0$ , then  $\sup_{\{p | \operatorname{Re}: p \geq 0\}} |\theta(p)| \leq M$ ;
4. If the function  $\Theta'(s)$  is bounded in the half-plane  $\operatorname{Re}: z \geq 0$ , then  $\theta$  is analytic in the half-plane  $\operatorname{Re}: p > 0$ .

*Proof.* 1. Let  $0 \leq p_1 \leq p_2$ . Since  $\Theta$  is monotone, we obtain

$$\theta(p_1) = \int_0^{\infty} \Theta(Kp_1) \mathcal{N}(K) dK \leq \int_0^{\infty} \Theta(Kp_2) \mathcal{N}(K) dK = \theta(p_2).$$

2. Let  $\varepsilon > 0$  and let  $K_\varepsilon$  be such that  $\int_{K_\varepsilon}^\infty \mathcal{N}(K) dK < \varepsilon$ . Then we get

$$\begin{aligned} \theta(p) &= \int_0^\infty \Theta(Kp)\mathcal{N}(K) dK \\ &= \int_0^{K_\varepsilon} \Theta(Kp)\mathcal{N}(K) dK + \int_{K_\varepsilon}^\infty \Theta(Kp)\mathcal{N}(K) dK \\ &\leq \int_0^{K_\varepsilon} \Theta(K_\varepsilon p)\mathcal{N}(K) dK + \int_{K_\varepsilon}^\infty \mathcal{N}(K) dK \\ &< \Theta(K_\varepsilon p) + \varepsilon < 2\varepsilon, \end{aligned}$$

whenever  $p > 0$  is sufficiently small. Hence  $\lim_{p \rightarrow 0^+} \theta(p) = 0$ .

Let  $\varepsilon > 0$  and let  $p > 0$ . Then from (8) we obtain

$$\begin{aligned} 1 &\geq \int_0^\infty \Theta(Kp)\mathcal{N}(K) dK = \int_{K_0}^\infty \Theta(Kp)\mathcal{N}(K) dK \\ &\geq \int_{K_0}^\infty \Theta(K_0 p)\mathcal{N}(K) dK \\ &= \Theta(K_0 p) \geq 1 - \varepsilon, \end{aligned}$$

whenever  $p > 0$  is big enough. Thus  $\lim_{p \rightarrow +\infty} \theta(p) = 1$ .

3. Let  $\text{Re}: p \geq 0$ . Then we have

$$|\theta(p)| \leq \int_0^\infty |\Theta(Kp)|\mathcal{N}(K) dK \leq M \int_0^\infty \mathcal{N}(K) dK = M.$$

4. Let  $\text{Re}: p_0 > 0$ . Then we have  $|\Theta'(Kp_0)Kp_0| \leq M$ , for all  $K > 0$ . Therefore the integral

$$I(p) = \int_0^\infty \Theta'(Kp)Kp\mathcal{N}(K) dK$$

converges uniformly in  $\{p \mid |p - p_0| < \text{Re}: p_0/2\}$  and  $\theta'(p) = I(p)/p$ . Thus  $\theta$  is analytic in the half-plane  $\text{Re}: p > 0$ .  $\square$

**3. General solution to the adsorption equation.** In this section we derive a formula for the solution to the adsorption equation. First we consider the Langmuir kernel and the case when the kernel is a

polynomial of Langmuir's kernel. Then passing to the limit when the degree of the polynomial tends to infinity, we get the solution in the general case.

**3.1 Langmuir's kernel and the Stieltjes integral equation.** If  $Q_1 = 1$  and  $Q_j = 0$ ,  $j > 1$ , then we get the Langmuir local isotherm

$$\Theta(Kp) = \frac{Kp}{1 + Kp}.$$

In this case equation (6) can be reduced to the Stieltjes integral equation. Indeed, put  $t = K$ ,  $\xi = 1/p$ ,  $\phi(t) = t\mathcal{N}(t)$ , and  $\Phi(\xi) = \theta(1/\xi)$ . Then from (6) we have

$$(11) \quad \Phi(\xi) = \int_0^\infty \frac{\phi(t)dt}{t + \xi},$$

where  $\Phi(\xi)$ ,  $\xi \geq 1$ , is a known function and the problem is to find  $\phi(t) \geq 0$ ,  $t \in [0, \infty)$ . Moreover  $\phi$  satisfies

$$(12) \quad \int_0^\infty \frac{\phi(t)dt}{t} = 1.$$

For the sake of simplicity we shall consider this problem in the class of continuous functions  $\phi$ . From (11) it follows that  $\Phi(\xi)$  is analytic in the complex plane cut along the ray  $L = \{\xi \mid \text{Re: } \xi \leq 0, \text{ Im: } \xi = 0\}$  and

$$(13) \quad \phi(x) = \lim_{y \downarrow 0} \frac{\Phi(-x - iy) - \Phi(-x + iy)}{2\pi i}, \quad x > 0,$$

see [17]. This solution to (11) was obtained by Stieltjes. To find the energy distribution function this relation was first used by Sips [14, 15].

**3.2 Polynomial kernel.** Now consider the case when the function  $Q(q)$  is a polynomial:

$$Q(q) = \sum_{j=1}^J Q_j q^j.$$



Then the kernel has the form

$$\Theta(Kp) = \sum_{j=1}^J Q_j \left( \frac{Kp}{1 + Kp} \right)^j.$$

Put

$$(14) \quad \mathcal{L}(\mathcal{N})(p) = \int_0^\infty \frac{Kp}{1 + Kp} \mathcal{N}(K) dK.$$

By Proposition 2 the function  $\mathcal{L}(\mathcal{N})(p)$  satisfies the following conditions

$$(15) \quad \lim_{p \rightarrow 0} \mathcal{L}(\mathcal{N})(p) = 0 \quad \text{and} \quad \lim_{p \rightarrow \infty} \mathcal{L}(\mathcal{N})(p) = 1.$$

Since  $\lim_{s \rightarrow \infty} \Theta(s) = 1$ , we have

$$\sum_{j=1}^J Q_j = 1.$$

Adsorption integral equation (6) takes the form

$$(16) \quad \theta(p) = \sum_{j=1}^J Q_j \int_0^\infty \left( \frac{Kp}{1 + Kp} \right)^j \mathcal{N}(K) dK.$$

Set

$$\mathcal{P}(\alpha) = \sum_{j=0}^{J-1} \frac{(-1)^j Q_{j+1}}{j!} \alpha(\alpha - 1) \cdots (\alpha - j + 1).$$

Let  $\alpha_l, l = \overline{1, L}$ , be different roots of the polynomial  $\mathcal{P}(\alpha)$  with multiplicities  $n_l, l = \overline{1, L}$ , respectively. Observe that  $\mathcal{P}(-1) = \sum_{j=0}^{J-1} Q_{j+1} = 1$ . Therefore,  $\alpha = -1$  is not a root of  $\mathcal{P}$ .

**Theorem 1.** *The function  $\mathcal{L}(\mathcal{N})(p)$  can be represented in the form*

$$(17) \quad \mathcal{L}(\mathcal{N})(p) = \sum_{l=1}^L \sum_{k=1}^{n_l} p(c_{lk} I_k(\alpha_l, p) + b_{lk} S_k(\alpha_l, p)),$$

where

$$c_{lk} = \frac{1}{(n_l - k)!} \frac{d^{n_l - k}}{d\alpha^{n_l - k}} \left( \frac{(\alpha - \alpha_l)^{n_l}}{\mathcal{P}(\alpha)} \right)_{\alpha = \alpha_l}, \quad k = \overline{1, n_l}, \quad l = \overline{1, L},$$

$$I_k(\alpha, p) = \frac{1}{(k-1)!} \int_1^p \left( \ln \frac{p}{r} \right)^{k-1} \left( \frac{p}{r} \right)^\alpha \frac{\theta(r) dr}{r^2},$$

$$S_k(\alpha, p) = (\ln p)^{k-1} p^\alpha,$$

and the constants  $b_{lk}$ ,  $k = \overline{1, n_l}$ ,  $l = \overline{1, L}$ , are uniquely determined by condition (15). If  $\operatorname{Re}: \alpha_l \neq -1$ ,  $l = \overline{1, L}$ , then

$$(18) \quad b_{lm} = (-1)^{k-m+1} \sum_{k=m}^{n_l} \frac{c_{lk}}{(k-1)!} \binom{k-1}{m-1} \\ \times \int_1^\infty (\ln r)^{k-m} \frac{\theta(r) dr}{r^{\alpha_l+2}}, \quad \operatorname{Re}: \alpha > -1$$

$$(19) \quad b_{lm} = (-1)^{k-m} \sum_{k=m}^{n_l} \frac{c_{lk}}{(k-1)!} \binom{k-1}{m-1} \\ \times \int_0^1 (\ln r)^{k-m} \frac{\theta(r) dr}{r^{\alpha_l+2}}, \quad \operatorname{Re}: \alpha < -1.$$

and the following representation holds

$$(20) \quad \mathcal{L}(\mathcal{N})(p) = \frac{\theta(\infty) - \theta(0)}{2} \\ + \frac{1}{2\pi i} \text{P.V.} \int_{-\infty}^{+\infty} \frac{1}{\gamma \mathcal{P}(-1+i\gamma)} \int_0^{+\infty} \left( \frac{p}{r} \right)^{i\gamma} d\theta(r) d\gamma,$$

where P.V. means an integral is in the sense of principal value.

*Remark.* By  $z^\alpha$  we mean the branch, single-valued in the plane cut along the negative real ray.

*Proof.* Consider the function

$$(21) \quad G(p) = \frac{1}{p} \mathcal{L}(\mathcal{N})(p).$$

Since

$$\frac{\partial^j G(p)}{\partial p^j} = (-1)^j j! \int_0^\infty \left( \frac{K}{1 + Kp} \right)^{j+1} \mathcal{N}(K) dK,$$

from (16) we see that the function  $G$  satisfies the Euler equation

$$(22) \quad \frac{\theta(p)}{p} = \sum_{j=0}^{J-1} \frac{(-1)^j Q_{j+1}}{j!} p^j G^{(j)}(p), \quad p > 0$$

and the boundary conditions

$$(23) \quad \lim_{p \rightarrow 0} pG(p) = 0 \quad \text{and} \quad \lim_{p \rightarrow \infty} pG(p) = 1,$$

see (15). The substitution  $t = \ln p$  transforms the Euler equation into a linear differential equation with constant coefficients. A general solution to (22) is given by

$$G(p) = \sum_{l=1}^L \sum_{k=1}^{n_l} (c_{lk} I_k(\alpha_l, p) + b_{lk} S_k(\alpha_l, p))$$

where  $b_{lk}$ ,  $k = \overline{1, n_l}$ ,  $l = \overline{1, L}$ , are arbitrary constants. From this we obtain (17).

We need two technical lemmas.

**Lemma 1.** *Let  $g$  be a solution to the homogeneous Euler equation*

$$(24) \quad 0 = \sum_{j=0}^{J-1} \frac{(-1)^j Q_{j+1}}{j!} p^j g^{(j)}(p), \quad p > 0.$$

1. *If  $\lim_{p \rightarrow 0} pg(p) = \lim_{p \rightarrow \infty} pg(p) = 0$ , then  $g \equiv 0$ .*
2. *If  $\text{Re}: \alpha_l \neq -1$ ,  $l = \overline{1, L}$ , and  $|pg(p)| \leq b$ ,  $p \geq 0$ , then  $g \equiv 0$ .*

*Proof.* The proof is elementary and follows from the formula

$$g(p) = \sum_{l=1}^L \sum_{k=1}^{n_l} b_{lk} (\ln p)^{k-1} p^{\alpha_l}. \quad \square$$

**Lemma 2.** *Assume that  $G(p)$  is a solution to (22) and the function  $pG(p)$ ,  $p \geq 0$ , is bounded. If  $\operatorname{Re}: \alpha_l \neq -1$ ,  $l = \overline{1, L}$ , then*

$$G(p) = \sum_{l=1}^L \sum_{k=1}^{n_l} (c_{lk} I_k(\alpha_l, p) + b_{lk} S_k(\alpha_l, p)),$$

where the constants  $b_{lk}$ ,  $k = \overline{1, n_l}$ ,  $l = \overline{1, L}$ , are given by (18) and (19).

*Proof.* Since  $\operatorname{Re}: \alpha_l \neq -1$ ,  $l = \overline{1, L}$ , the constants  $b_{lk}$ ,  $k = \overline{1, n_l}$ ,  $l = \overline{1, L}$ , can be easily found. Indeed, observe that

$$(25) \quad G(p) = \sum_{l=1}^L \sum_{m=1}^{n_l} \left[ \sum_{k=m}^{n_l} \frac{c_{lk}}{(k-1)!} \binom{k-1}{m-1} \times \int_1^p (-\ln r)^{k-m} \frac{\theta(r) dr}{r^{\alpha_l+2}} + b_{lm} \right] (\ln p)^{m-1} p^{\alpha_l}.$$

Since the integrals

$$\int_1^\infty (\ln r)^\beta \frac{\theta(r) dr}{r^{\alpha+2}}, \quad \operatorname{Re}: \alpha > -1$$

and

$$\int_0^1 (\ln r)^\beta \frac{\theta(r) dr}{r^{\alpha+2}}, \quad \operatorname{Re}: \alpha < -1$$

exist, from the boundedness of the function  $pG(p)$  and (25) we get (18) and (19).  $\square$

*End of the proof of Theorem 1.* The uniqueness follows from Lemma 1. If  $\operatorname{Re}: \alpha_l \neq -1$ ,  $l = \overline{1, L}$ , then from Lemma 2 we obtain (18) and (19).

It remains to prove (20). Suppose that all roots of the characteristic polynomial are simple. Then substituting (18) and (19) for  $b_{lk}$  in (17), we obtain

$$\mathcal{L}(\mathcal{N})(p) = \sum_{l \in \mathcal{J}^-} \frac{p^{\alpha_l+1}}{\mathcal{P}'(\alpha_l)} \int_0^p \frac{\theta(r) dr}{r^{\alpha_l+2}} - \sum_{l \in \mathcal{J}^+} \frac{p^{\alpha_l+1}}{\mathcal{P}'(\alpha_l)} \int_p^\infty \frac{\theta(r) dr}{r^{\alpha_l+2}},$$

where  $\mathcal{J}^- = \{l \mid \text{Re: } \alpha_l < -1\}$  and  $\mathcal{J}^+ = \{l \mid \text{Re: } \alpha_l > -1\}$ . Integrating by parts, we get

$$\begin{aligned} \mathcal{L}(\mathcal{N})(p) &= \sum_{l \in \mathcal{J}^-} \frac{1}{\mathcal{P}'(\alpha_l)(\alpha_l + 1)} \left[ -\theta(p) + \int_0^p \left(\frac{p}{r}\right)^{\alpha_l+1} d\theta(r) \right] \\ &\quad - \sum_{l \in \mathcal{J}^+} \frac{1}{\mathcal{P}'(\alpha_l)(\alpha_l + 1)} \left[ \theta(p) + \int_p^\infty \left(\frac{p}{r}\right)^{\alpha_l+1} d\theta(r) \right] \\ &= \sum_{l \in \mathcal{J}^-} \text{res}_{\alpha=\alpha_l} \frac{\delta_p^-(\alpha)}{\mathcal{P}(\alpha)} - \sum_{l \in \mathcal{J}^+} \text{res}_{\alpha=\alpha_l} \frac{\delta_p^+(\alpha)}{\mathcal{P}(\alpha)}, \end{aligned}$$

where

$$\begin{aligned} \delta_p^-(\alpha) &= \frac{1}{\alpha + 1} \left[ -\theta(p) + \int_0^p \left(\frac{p}{r}\right)^{\alpha+1} d\theta(r) \right], \\ \delta_p^+(\alpha) &= \frac{1}{\alpha + 1} \left[ \theta(p) + \int_p^\infty \left(\frac{p}{r}\right)^{\alpha+1} d\theta(r) \right]. \end{aligned}$$

The last equality can be also written in the following form

$$\mathcal{L}(\mathcal{N})(p) = \frac{1}{2\pi i} \int_{\Gamma_\rho^-} \frac{\delta_p^-(\alpha)}{\mathcal{P}(\alpha)} d\alpha - \frac{1}{2\pi i} \int_{\Gamma_\rho^+} \frac{\delta_p^+(\alpha)}{\mathcal{P}(\alpha)} d\alpha,$$

where the contours  $\Gamma_\rho^\pm$  are given by

$$\begin{aligned} \Gamma_\rho^- &= \{\alpha \mid |\alpha + 1| = 1/\rho, \text{Re: } \alpha \leq -1\} \\ &\quad \cup \{\alpha \mid \text{Re: } \alpha = -1, \text{Im: } \alpha \in [-\rho, -1/\rho] \cup [1/\rho, \rho]\} \\ &\quad \cup \{\alpha \mid |\alpha + 1| = \rho, \text{Re: } \alpha \leq -1\} \end{aligned}$$

and

$$\begin{aligned} \Gamma_\rho^+ &= \{\alpha \mid |\alpha + 1| = 1/\rho, \text{Re: } \alpha \geq -1\} \\ &\quad \cup \{\alpha \mid \text{Re: } \alpha = -1, \text{Im: } \alpha \in [-\rho, -1/\rho] \cup [1/\rho, \rho]\} \\ &\quad \cup \{\alpha \mid |\alpha + 1| = \rho, \text{Re: } \alpha \geq -1\}, \end{aligned}$$

and  $\rho > 0$  is big enough. Passing to the limit as  $\rho \rightarrow \infty$ , we obtain

$$\begin{aligned}
\mathcal{L}(\mathcal{N})(p) &= \frac{1}{2\pi} \lim_{\rho \rightarrow \infty} \left[ \int_{3\pi/2}^{\pi/2} \frac{1}{\mathcal{P}(-1+e^{i\lambda}/\rho)} \left[ -\theta(p) + \int_0^p \left(\frac{p}{r}\right)^{e^{i\lambda}/\rho} d\theta(r) \right] d\lambda \right. \\
&\quad \left. - \int_{\pi/2}^{-\pi/2} \frac{1}{\mathcal{P}(-1+e^{i\lambda}/\rho)} \left[ \theta(p) + \int_p^\infty \left(\frac{p}{r}\right)^{e^{i\lambda}/\rho} d\theta(r) \right] d\lambda \right] \\
&+ \frac{1}{2\pi i} \lim_{\rho \rightarrow \infty} \left[ \int_{-1-i\rho}^{-1-i/\rho} \frac{1}{\mathcal{P}(\alpha)(\alpha+1)} \int_0^\infty \left(\frac{p}{r}\right)^{\alpha+1} d\theta(r) d\alpha \right. \\
&\quad \left. + \int_{-1+i/\rho}^{-1+i\rho} \frac{1}{\mathcal{P}(\alpha)(\alpha+1)} \int_0^\infty \left(\frac{p}{r}\right)^{\alpha+1} d\theta(r) d\alpha \right] \\
&= \frac{\theta(\infty) - \theta(0)}{2} \\
&+ \frac{1}{2\pi i} \text{P.V.} \int_{-1-i\infty}^{-1+i\infty} \frac{1}{\mathcal{P}(\alpha)(\alpha+1)} \int_0^\infty \left(\frac{p}{r}\right)^{\alpha+1} d\theta(r) d\alpha \\
&= \frac{\theta(\infty) - \theta(0)}{2} \\
&+ \frac{1}{2\pi i} \text{P.V.} \int_{-\infty}^{+\infty} \frac{1}{\gamma \mathcal{P}(-1+i\gamma)} \int_0^{+\infty} \left(\frac{p}{r}\right)^{i\gamma} d\theta(r) d\gamma.
\end{aligned}$$

If the roots of the characteristic polynomial are not simple, the polynomial can be approximated by polynomials with simple roots and taking the limit we get (20).  $\square$

**3.3 General case.** Here we show that the formula for  $\mathcal{L}(\mathcal{N})(p)$  obtained in the previous section can be also used when  $\Theta(Kp)$  is given by an infinite series (9). In this case  $\mathcal{P}(\alpha)$  is a series

$$\mathcal{P}(\alpha) = \sum_{j=0}^{\infty} \frac{(-1)^j Q_{j+1}}{j!} \alpha(\alpha-1) \cdots (\alpha-j+1).$$

The series of this type are known as Newton series. We shall call  $\mathcal{P}$  a characteristic function. We say that the characteristic function is well defined if the Newton series converges for  $\alpha$  with  $\text{Im } \alpha = -1$ , and is different from zero.

Now let us prove the main result.

**Theorem 2.** Assume that

1. the series  $\sum_{j=1}^{\infty} j|Q_j|$  converges,
2. there exists the integral

$$\int_0^{\infty} \ln K \mathcal{N}(K) dK,$$

3. there exist a constant  $c > 0$  and a sequence of polynomials

$$\mathcal{P}_J(\alpha) = \sum_{j=0}^{J-1} \frac{(-1)^j Q_{j+1}^{(J)}}{j!} \alpha(\alpha - 1) \cdots (\alpha - j + 1)$$

such that  $|\mathcal{P}_J(-1 + i\gamma)| > c(1 + |\gamma|)$ , for all  $\gamma \in (-\infty, +\infty)$ , and

$$\lim_{J \rightarrow \infty} \sum_{j=1}^{\infty} j|Q_j^{(J)} - Q_j| = 0,$$

where  $Q_j^{(J)} = 0$ ,  $j > J$ .

Then the characteristic function  $\mathcal{P}(\alpha)$  is well defined for  $\alpha$  with  $\text{Re } \alpha = -1$  and

(26)

$$\mathcal{L}(\mathcal{N})(p) = \frac{\theta(\infty) - \theta(0)}{2} + \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \int_0^{+\infty} \frac{1}{\gamma} \left( \frac{(p/r)^{i\gamma}}{\mathcal{P}(-1 + i\gamma)} - 1 \right) d\theta(r) d\gamma.$$

*Remark.* The second condition of the theorem is equivalent with the existence of a finite energy distribution first moment:

$$\int_0^{\infty} EN(E) dE < \infty.$$

*Proof.* First show that the characteristic function  $\mathcal{P}(\alpha)$  is well defined. Indeed, since  $\sum_{j=1}^{\infty} j|Q_j| < +\infty$  the Newton series

$$\mathcal{P}(\alpha) = \sum_{j=0}^{\infty} \frac{(-1)^j Q_{j+1}}{j!} \alpha(\alpha - 1) \cdots (\alpha - j + 1)$$

converges for  $\alpha = -2$ . This implies the convergence for all  $\alpha$  satisfying  $\operatorname{Re}\alpha > -2$ , see [7], for example.

Without loss of generality all roots of the polynomials  $\mathcal{P}_J(\alpha)$  are different. Denote them by  $\alpha_{J,l}$ ,  $l = \overline{1, J-1}$ . Consider the function

$$G_J(p) = \sum_{l \in \mathcal{J}_J^-} \frac{p^{\alpha_{J,l}+1}}{\mathcal{P}'_J(\alpha_{J,l})} \int_0^p \frac{\theta(r)dr}{r^{\alpha_{J,l}+2}} - \sum_{l \in \mathcal{J}_J^+} \frac{p^{\alpha_{J,l}+1}}{\mathcal{P}'_J(\alpha_{J,l})} \int_p^\infty \frac{\theta(r)dr}{r^{\alpha_{J,l}+2}},$$

where  $\mathcal{J}_J^- = \{l \mid \operatorname{Re} \alpha_{J,l} < -1\}$  and  $\mathcal{J}_J^+ = \{l \mid \operatorname{Re} \alpha_{J,l} > -1\}$ . It satisfies the Euler equation

$$(27) \quad \frac{\theta(p)}{p} = \sum_{j=0}^{J-1} \frac{(-1)^j Q_{j+1}^{(J)}}{j!} p^j G_J^{(j)}(p), \quad p > 0,$$

see the proof of Theorem 1. Since

$$\left| \int_0^p \left(\frac{p}{r}\right)^{\alpha_{J,l}+1} \frac{\theta(r)dr}{r} \right| \leq \int_0^p \left(\frac{p}{r}\right)^{\operatorname{Re}\alpha_{J,l}+1} \frac{\theta(r)dr}{r} = \frac{1}{1 - \operatorname{Re}\alpha_{J,l}},$$

$$l \in \mathcal{J}_J^-,$$

and

$$\left| \int_p^\infty \left(\frac{p}{r}\right)^{\alpha_{J,l}+1} \frac{\theta(r)dr}{r} \right| \leq \int_p^\infty \left(\frac{p}{r}\right)^{\operatorname{Re}\alpha_{J,l}+1} \frac{\theta(r)dr}{r} = \frac{1}{1 + \operatorname{Re}\alpha_{J,l}},$$

$$l \in \mathcal{J}_J^+,$$

we see that there exists a constant  $b > 0$  such that

$$(28) \quad |pG_J(p)| \leq b, \quad p \geq 0.$$

From Lemma 1 we conclude that  $G_J(p)$  is a unique solution to (27) satisfying (28). Invoking Lemma 2 and arguing as in the last part of the proof of Theorem 1, we obtain

$$pG_J(p) = \frac{\theta(\infty) - \theta(0)}{2} + \frac{1}{2\pi i} \text{P.V.} \int_{-\infty}^{+\infty} \frac{1}{\gamma \mathcal{P}_J(-1 + i\gamma)} \int_0^{+\infty} \left(\frac{p}{r}\right)^{i\gamma} d\theta(r) d\gamma.$$



Put

$$g_J(p) = G(p) - G_J(p)$$

and

$$\begin{aligned} \sigma_J(p) &= \sum_{j=0}^{\infty} \frac{(-1)^j (Q_{j+1}^{(J)} - Q_{j+1})}{j!} p^{j+1} G^{(j)}(p) \\ &= \sum_{j=1}^{\infty} (Q_j^{(J)} - Q_j) \int_0^{\infty} \left( \frac{Kp}{1 + Kp} \right)^j \mathcal{N}(K) dK. \end{aligned}$$

Then we have

$$\frac{\sigma_J(p)}{p} = \sum_{j=0}^{J-1} \frac{(-1)^j Q_{j+1}^{(J)}}{j!} p^j g^{(j)}(p), \quad p > 0.$$

Moreover  $|pg_J(p)| < b_J, p \geq 0$ , where  $b_J > 0$  is a constant. By Lemma 1 these conditions uniquely determine the function  $g_J(p)$ . Applying Lemma 2, as above we get

$$\begin{aligned} pg_J(p) &= \frac{\sigma_J(\infty) - \sigma_J(0)}{2} \\ &\quad + \frac{1}{2\pi i} \text{P.V.} \int_{-\infty}^{+\infty} \frac{1}{\gamma \mathcal{P}_J(-1 + i\gamma)} \int_0^{+\infty} \left( \frac{p}{r} \right)^{i\gamma} d\sigma_J(r) d\gamma. \end{aligned}$$

To estimate the integral

$$I(p) = \text{P.V.} \int_{-\infty}^{+\infty} \frac{1}{\gamma \mathcal{P}_J(-1 + i\gamma)} \int_0^{+\infty} \left( \frac{p}{r} \right)^{i\gamma} d\sigma_J(r) d\gamma$$

observe that it can be represented as a sum of three integrals

$$I(p) = I_1(p) + I_2(p) + I_3(p),$$

where

$$\begin{aligned} I_1(p) &= \text{P.V.} \int_{-1}^1 \frac{1}{\gamma \mathcal{P}_J(-1 + i\gamma)} \int_0^{+\infty} \left( \frac{p}{r} \right)^{i\gamma} d\sigma_J(r) d\gamma, \\ I_2(p) &= \int_{-\infty}^{-1} \frac{1}{\gamma \mathcal{P}_J(-1 + i\gamma)} \int_0^{+\infty} \left( \frac{p}{r} \right)^{i\gamma} d\sigma_J(r) d\gamma, \end{aligned}$$

and

$$I_3(p) = \int_1^{+\infty} \frac{1}{\gamma \mathcal{P}_J(-1+i\gamma)} \int_0^{+\infty} \left(\frac{p}{r}\right)^{i\gamma} d\sigma_J(r) d\gamma.$$

The integrals  $I_2(p)$  and  $I_3(p)$  satisfy the inequality

$$\begin{aligned} (29) \quad |I_{2,3}(p)| &\leq \int_{-\infty}^{+\infty} \frac{d\gamma}{|\mathcal{P}_J(-1+i\gamma)|} \int_0^\infty |d\sigma_J(r)| \\ &\leq \int_{-\infty}^{+\infty} \frac{d\gamma}{|\mathcal{P}_J(-1+i\gamma)| \max\{1, |\gamma|\}} \\ &\quad \times \int_0^\infty \sum_{j=1}^\infty |Q_j^{(j)} - Q_j| d \left( \int_0^\infty \left(\frac{Kp}{1+Kp}\right)^j \mathcal{N}(K) dK \right) \\ &= \int_{-\infty}^{+\infty} \frac{d\gamma}{c(1+|\gamma|) \max\{1, |\gamma|\}} \sum_{j=1}^\infty |Q_j^{(j)} - Q_j|. \end{aligned}$$

To estimate the integral  $I_1(p)$  note that  $\text{P.V.} \int_{-\infty}^{+\infty} d\gamma/\gamma = 0$  and therefore

$$\begin{aligned} I_1(p) &= \text{P.V.} \int_{-1}^1 \frac{1}{\gamma} \int_0^\infty \left( \frac{(p/r)^{i\gamma}}{\mathcal{P}_J(-1+i\gamma)} - \frac{1}{\mathcal{P}_J(-1)} \right) d\sigma_J(r) d\gamma \\ &= I^*(p) + I^{**}(p), \end{aligned}$$

where

$$I^*(p) = \text{P.V.} \int_{-1}^1 \frac{1}{\gamma} \int_0^\infty \frac{(p/r)^{i\gamma} - 1}{\mathcal{P}_J(-1+i\gamma)} d\sigma_J(r) d\gamma$$

and

$$I^{**}(p) = \text{P.V.} \int_{-1}^1 \frac{1}{\gamma} \int_0^\infty \left( \frac{1}{\mathcal{P}_J(-1+i\gamma)} - \frac{1}{\mathcal{P}_J(-1)} \right) d\sigma_J(r) d\gamma.$$

Since

$$\begin{aligned} \left| \frac{1}{\gamma} \left( \left(\frac{p}{r}\right)^{i\gamma} - 1 \right) \right| &= \left| \frac{1}{\gamma} \int_0^\gamma \left( \frac{d}{d\omega} \left(\frac{p}{r}\right)^{i\omega} \right) d\omega \right| \\ &= \left| \frac{1}{\gamma} \int_0^\gamma \left( -i \left(\frac{p}{r}\right)^{i\omega} \ln r \right) d\omega \right| \leq |\ln r|, \end{aligned}$$

we have

$$|I^*(p)| \leq \int_{-1}^1 \frac{d\gamma}{|\mathcal{P}_J(-1+i\gamma)|} \int_0^\infty \ln r \, d\sigma_J(r).$$

Observe that

$$\begin{aligned} \int_0^\infty \ln r \, d\sigma_J(r) &= \int_0^\infty \ln r \sum_{j=1}^\infty (Q_j^{(J)} - Q_j) d \int_0^\infty \left(\frac{Kr}{1+Kr}\right)^j \mathcal{N}(K) dK \\ &= \sum_{j=1}^\infty (Q_j^{(J)} - Q_j) \int_0^\infty \left[ \int_0^\infty \ln r \, d \left(\frac{Kr}{1+Kr}\right)^j \right] \mathcal{N}(K) dK. \end{aligned}$$

We need the following auxiliary estimate.

**Lemma 3.** *The following inequality holds*

$$\left| \int_0^\infty \ln r \, d \left(\frac{Kr}{1+Kr}\right)^n \right| \leq 1 + n \ln 2 + \ln K.$$

*Proof.* Indeed, we have

$$\begin{aligned} (30) \quad \int_0^\infty \ln r \, d \left(\frac{Kr}{1+Kr}\right)^n &= \int_0^\infty \ln(Kr) d \left(\frac{Kr}{1+Kr}\right)^n - \ln K \int_0^\infty d \left(\frac{Kr}{1+Kr}\right)^n \\ &= \int_0^\infty \ln s \, d \left(\frac{s}{1+s}\right)^n - \ln K. \end{aligned}$$

This integral can be represented as

$$\begin{aligned} \int_0^\infty \ln s \, d \left(\frac{s}{1+s}\right)^n &= \int_0^1 \ln s \, d \left(\frac{s}{1+s}\right)^n \\ &\quad + \int_1^\infty \ln s \, d \left( \left(\frac{s}{1+s}\right)^n - 1 \right). \end{aligned}$$

Integrating by parts we obtain

$$\begin{aligned} \int_0^\infty \ln s \, d \left(\frac{s}{1+s}\right)^n &= - \int_0^1 \frac{1}{s} \left(\frac{s}{1+s}\right)^{n-1} \frac{ds}{1+s} \\ &\quad + \int_1^\infty \frac{1}{s} \left( 1 - \left(1 - \frac{1}{1+s}\right)^n \right) ds. \end{aligned}$$

Obviously

$$(31) \quad \left| \int_0^1 \frac{1}{s} \left( \frac{s}{1+s} \right)^{n-1} \frac{ds}{1+s} \right| \leq 1.$$

To estimate the second integral observe that

$$\left( 1 - \frac{1}{1+s} \right)^n \geq 1 - \frac{n}{1+s}$$

(Bernoulli's inequality). Therefore we have

$$\int_1^\infty \frac{1}{s} \left( 1 - \left( 1 - \frac{1}{1+s} \right)^n \right) ds \leq n \int \frac{ds}{s(1+s)} = n \ln 2.$$

Combining this with (30) and (31) we obtain the result.  $\square$

Invoking the lemma we obtain

$$\begin{aligned} \left| \int_0^\infty \ln r d\sigma_J(r) \right| &\leq \sum_{j=1}^\infty |Q_j^{(J)} - Q_j| \int_0^\infty (1 + j \ln 2 + \ln K) \mathcal{N}(K) dK \\ &\leq (\text{const}) \sum_{j=1}^\infty j |Q_j^{(J)} - Q_j|. \end{aligned}$$

Thus we have

$$(32) \quad |I^*(p)| \leq (\text{const}) \int_{-1}^1 \frac{d\gamma}{c(1+|\gamma|)} \sum_{j=1}^\infty j |Q_j^{(J)} - Q_j|.$$

To estimate the integral  $I^{**}(p)$  observe that

$$\begin{aligned} \mathcal{P}'_J(-1+i\omega) &= i \sum_{j=0}^{J-1} \frac{(-1)^j Q_{j+1}^{(J)}}{j!} \\ &\quad \times \sum_{k=0}^{j-1} (i\omega-1) \cdots (i\omega-k)(i\omega-k-2) \cdots (i\omega-j). \end{aligned}$$

From this we obtain

$$\begin{aligned} |\mathcal{P}'_J(-1 + i\omega)| &\leq \sum_{j=0}^{J-1} \frac{|Q_{j+1}^{(J)}|}{j!} \sum_{k=0}^{j-1} 2 \cdot 3 \cdot \dots \cdot j \\ &\leq \sum_{j=1}^J j|Q_j^{(J)}| \leq \sum_{j=1}^{\infty} j|Q_j^{(J)} - Q_j| + \sum_{j=1}^{\infty} j|Q_j|. \end{aligned}$$

Therefore we get

$$\begin{aligned} |I^{**}(p)| &\leq \left| \int_{-1}^1 \left( \frac{1}{\gamma \mathcal{P}_J(-1 + i\gamma)} - \frac{1}{\mathcal{P}_J(-1)} \right) d\gamma \right| \left| \int_0^{\infty} d\sigma_J(r) \right| \\ &\leq \left| \int_{-1}^1 \frac{\gamma^{-1} \int_0^{\gamma} \mathcal{P}'_J(-1 + i\omega) d\omega}{\mathcal{P}_J(-1 + i\gamma) \mathcal{P}_J(-1)} \right| \sum_{j=1}^{\infty} |Q_j^{(J)} - Q_j| \\ &\leq \int_{-1}^1 \frac{d\gamma}{2c^2(1+|\gamma|)} \left( \sum_{j=1}^{\infty} j|Q_j^{(J)} - Q_j| + \sum_{j=1}^{\infty} j|Q_j| \right) \sum_{j=1}^{\infty} |Q_j^{(J)} - Q_j|. \end{aligned}$$

Combining this with (32) we obtain

$$|I_1(p)| \leq (\text{const}) \sum_{j=1}^{\infty} j|Q_j^{(J)} - Q_j|.$$

From this and (29) we see that  $|pg_J(p)|$  tends to zero as  $J$  goes to infinity. Passing to the limit as  $J \rightarrow \infty$  in the equality

$$\begin{aligned} pG(p) = pg_J(p) + pG_J(p) &= \frac{\sigma_J(\infty) - \sigma_J(0)}{2} + \frac{\theta(\infty) - \theta(0)}{2} \\ &\quad + \frac{1}{2\pi i} \int_{-\infty}^{+\infty} \int_0^{+\infty} \frac{1}{\gamma} \left( \frac{(p/r)^{i\gamma}}{\mathcal{P}_J(-1 + i\gamma)} - \frac{1}{\mathcal{P}_J(-1)} \right) d(\sigma_J(r) + \theta(r)) d\gamma \end{aligned}$$

we obtain (26). This ends the proof.  $\square$

**4. Approximate solutions to the adsorption integral equation.** In this section we construct some approximations for solutions to the adsorption integral equation. We assume that the global isotherm  $\theta$  is known only at a sequence of points  $p_l > 0, l = 1, 2, \dots$ . As it will be

clear from our consideration this information is enough to reconstruct the function  $\theta(p)$  in the half-plane  $\text{Re}: p > 0$ . Using the results of the previous section one can find the function  $\mathcal{L}(\mathcal{N})(p)$ ,  $p > 0$ . Then it remains to solve the Stieltjes equation in order to find the distribution function  $\mathcal{N}$ . To this end we have to know  $\mathcal{L}(\mathcal{N})(p)$  in the complex plane cut along the negative real ray. We reduce the function  $\theta$  reconstruction problem and the solution of the Stieltjes equation to a problem of complex analytic continuation with prescribed bound. The main feature of the approach presented here is the use of condition (7) to derive bounds for the Taylor coefficient of the analytic function under consideration. This allows to reduce the analytic continuation problem to a sequence of mathematical programming problems, see Theorem 3.

**4.1 A series expansion for  $\theta(p)$ .** Consider the Möbius mapping

$$\zeta = \frac{p-1}{p+1}.$$

It maps the half-plane  $\text{Re}: p > 0$  onto the unit disk  $K = \{\zeta \mid |\zeta| < 1\}$  and the positive real ray on the disk's diameter,  $(-1, 1)$ . The inverse of  $\zeta = \zeta(p)$  is given by

$$p = \frac{1+\zeta}{1-\zeta}.$$

The function  $\theta(1 + \zeta/1 - \zeta)$  is analytic in  $K$  and

$$\sup_{\zeta \in K} \left| \theta \left( \frac{1+\zeta}{1-\zeta} \right) \right| \leq M.$$

Hence

$$\theta \left( \frac{1+\zeta}{1-\zeta} \right) = \sum_{k=0}^{\infty} \theta_k \zeta^k, \quad |\theta| < 1,$$

and from the Cauchy inequality we have  $|\theta_k| \leq M$ ,  $k = 1, 2, \dots$

**4.2 A change of variables in the Stieltjes equation.** Consider the conformal mapping

$$w = \frac{\sqrt{p}-1}{\sqrt{p}+1},$$

where by  $\sqrt{p}$  we mean the branch satisfying  $\sqrt{1} = 1$ . It maps the plane cut along  $L = \{p \mid \text{Re}: p \leq 0, \text{Im}: p = 0\}$  onto the unit disk  $K = \{w \mid |w| < 1\}$ . The “upper” side of  $L$ ,  $L^+ = \{p + i0\}$ , is transformed into the set  $\Gamma^+ = \{w \mid |w| = 1, \text{Im } w > 0\}$  and the “lower” side of  $L$ ,  $L^- = \{p - i0\}$ , is mapped on the set  $\Gamma^- = \{w \mid |w| = 1, \text{Im } w < 0\}$ . Finally the image of the ray  $-L$  is the disk’s diameter,  $(-1, 1)$ . The inverse of  $w = w(p)$  is given by

$$(34) \quad p = \left( \frac{1+w}{1-w} \right)^2.$$

In the complex plane  $w$  integral equation (11) has the form

$$(35) \quad \Psi(w) = - \int_{\Gamma^+} \mathcal{K}(w, \tau) \psi(\tau) d\tau, \quad -1 < w < 1,$$

where

$$\Psi(w) = \Phi \left( \left( \frac{1-w}{1+w} \right)^2 \right), \quad \psi(\tau) = \phi \left( - \left( \frac{1-\tau}{1+\tau} \right)^2 \right),$$

and

$$\mathcal{K}(w, \tau) = \left( \frac{1+w}{1+\tau} \right) \left( \frac{1}{w-\tau} + \frac{1}{1-\tau w} \right).$$

**4.3 Series expansions for  $\Psi$  and  $\phi$ .** If  $|w| < 1$  and  $|\tau| = 1$ , we can represent  $\mathcal{K}(w, \tau)$  in the following form

$$\mathcal{K}(w, \tau) = \left( \frac{1+w}{1+\tau} \right) \left( - \frac{1}{\tau} \left( 1 + \frac{w}{\tau} + \frac{w^2}{\tau^2} + \dots \right) + \left( 1 + \tau w + \tau^2 w^2 + \dots \right) \right).$$

Combining this with (35), we obtain

$$(36) \quad \Psi(w) = - \int_{\Gamma^+} \frac{\tau-1}{\tau(\tau+1)} \psi(\tau) d\tau - \sum_{k=1}^{\infty} \left( \int_{\Gamma^+} (\tau^{k-1} - \tau^{-k-1}) \psi(\tau) d\tau \right) w^k.$$

Putting  $\tau = e^{i\nu}$ ,  $\nu \in [0, \pi]$ , from (36) we get

$$(37) \quad \Psi(w) = \pi \sum_{k=0}^{\infty} b_k w^k,$$

where

$$b_0 = \frac{1}{\pi} \int_0^\pi \frac{1 - \cos \nu}{2} \mathcal{N} \left( \frac{1 - \cos \nu}{1 + \cos \nu} \right) d \left( \frac{1 - \cos \nu}{1 + \cos \nu} \right)$$

and

$$\begin{aligned} b_k &= \frac{1}{\pi} \int_0^\pi \sin k\nu \sin \nu \mathcal{N} \left( \frac{1 - \cos \nu}{1 + \cos \nu} \right) d \left( \frac{1 - \cos \nu}{1 + \cos \nu} \right) \\ &= \frac{2}{\pi} \int_0^\pi \sin k\nu \left( \frac{1 - \cos \nu}{1 + \cos \nu} \right) \mathcal{N} \left( \frac{1 - \cos \nu}{1 + \cos \nu} \right) d\nu \\ &= \frac{2}{\pi} \int_0^\pi \sin k\nu \phi \left( \frac{1 - \cos \nu}{1 + \cos \nu} \right) d\nu, \quad k = 1, 2, \dots \end{aligned}$$

The jump relation (13) now can be rewritten as

$$\psi(w) = \lim_{|w| \uparrow 1, \text{Im}: w > 0} \frac{\Psi(\bar{w}) - \Psi(w)}{2\pi i}.$$

Setting  $w = \rho e^{i\mu}$ ,  $\rho > 0$ ,  $\mu \in (0, \pi)$ , from (37) we obtain

$$(38) \quad \varphi(\mu) = \phi \left( \frac{1 - \cos \mu}{1 + \cos \mu} \right) = - \lim_{\rho \uparrow 1} \sum_{k=1}^{\infty} b_k \rho^k \sin k\mu.$$

Thus the function  $-\varphi$  is a limit of the Abel means of its Fourier sine series. Comparing (37) and (38), we see that the sine Fourier coefficients of  $-\varphi$  are the Taylor coefficients of  $\Psi$  divided by  $\pi$ .

The approximation techniques presented below are based on the following estimates for the coefficients  $b_k$ ,  $k = 1, 2, \dots$ ,

$$(39) \quad \begin{aligned} |b_k| &\leq \frac{1}{\pi} \int_0^\pi \mathcal{N} \left( \frac{1 - \cos \nu}{1 + \cos \nu} \right) d \left( \frac{1 - \cos \nu}{1 + \cos \nu} \right) \\ &= \frac{1}{\pi} \int_0^\infty \mathcal{N}(K) dK = \frac{1}{\pi}, \quad k = 1, 2, \dots \end{aligned}$$

**4.4 Approximation with constraints.** From the previous consideration we see that the reconstruction of the function  $\theta$  and solution



of the Stieltjes equation can be reduced to the problem of complex analytic continuation of a function, analytic in the unit disk, with prescribed bounds for the Taylor coefficients. Here we present a method, which allows to get an approximate solution to this problem stable with respect to small perturbations of the data.

Consider a function  $f$  analytic in the unit disk  $K = \{w \mid |w| < 1\}$ . The function  $f$  can be written as

$$f(w) = \sum_{k=0}^{\infty} a_k w^k, \quad |w| < 1.$$

We assume that

$$(40) \quad |a_k| \leq d_k, \quad k = 0, 1, 2, \dots$$

Let  $\{z_k\}_{k=0}^{\infty}$  be a sequence of complex numbers. By  $\vec{z}_n$  we shall denote the  $n$ -dimensional vector consisting of the first  $n$  terms of the sequence:  $\vec{z}_n = (z_0, z_1, \dots, z_{n-1})$ . By  $V_n^m(\vec{z}_n)$  we denote the  $m$ -norm in the  $n$ -dimensional space:

$$V_n^m(\vec{z}_n) = \left( \sum_{k=0}^{n-1} |z_k|^m \right)^{1/m}, \quad m = 1, 2, \dots,$$

and for  $m = \infty$  we put

$$V_n^\infty(\vec{z}_n) = \max_{k=0, n-1} |z_k|.$$

Let  $\{A_k\}_{k=0}^{\infty}$  be a sequence of complex numbers. Define the polynomials

$$P(w, \vec{A}_n) = \sum_{k=0}^{n-1} A_k w^k.$$

Consider two sequences  $\{w_k\}_{k=0}^{\infty}$  and  $\{f_k\}_{k=0}^{\infty}$ . We assume that  $|w_k| \leq r < 1$ . Let  $\bar{n}(n)$  be a sequence of non-negative integers satisfying  $\bar{n}(n) \geq n, n = 0, 1, \dots$ . Put

$$\vec{P}(\vec{A}_n) = (P(w_0, \vec{A}_n), P(w_1, \vec{A}_n), \dots, P(w_{\bar{n}(n)-1}, \vec{A}_n))$$

and

$$\vec{f}_n = (f(w_0), f(w_1), \dots, f(w_{\bar{n}(n)-1})).$$

Here the points  $w_k$ ,  $k = 0, 1, \dots$ , are the points where we know approximate values  $f_k$ ,  $k = 0, 1, \dots$ , of the function  $f$ . These values are, in general, different from the values  $f(w_k)$ ,  $k = 0, 1, \dots$ . Put  $\vec{A}_n = (a_0, a_1, \dots, a_{n-1})$ . Our aim is to find the coefficients  $a_k$ ,  $k = 0, 1, \dots$ . To this end we construct approximations of the function  $f$  by polynomials with coefficients satisfying restrictions (40).

Let  $m$  be a positive integer or  $\infty$ . Consider the following optimization problem

$$(41) \quad \text{minimize } \left\{ V_{\bar{n}(n)}^m(\vec{P}(\vec{A}_n) - \vec{f}_{\bar{n}(n)}) \mid |A_k| \leq d_k, k = \overline{0, n-1} \right\}.$$

The solution to this problem we denote by  $\vec{A}_n = (\hat{A}_0, \hat{A}_1, \dots, \hat{A}_{n-1})$ .

**Theorem 3.** *Assume that*

1.  $\lim_{n \rightarrow \infty} \sqrt{\bar{n}(n)} \sum_{k=n+1}^{\infty} d_k \rho^k = 0$ , for all  $\rho \in [0, 1)$ ,
2.  $\lim_{n \rightarrow \infty} V_n^m(\vec{f}_n - \vec{f}_n) = 0$ .

*Then the polynomials  $P(w, \vec{A}_n)$  converge uniformly inside the circle  $K = \{w \mid |w| < 1\}$  to the function  $f(w)$  as  $n$  goes to infinity.*

*Proof.* Let  $l$  and  $n$  be positive integers satisfying  $n \geq l$ . Then we have

$$\begin{aligned} |P(w_l, \vec{A}_n) - f(w_l)| &\leq V_{\bar{n}(n)}^m(\vec{P}(\vec{A}_n) - \vec{f}_{\bar{n}(n)}) \\ &\leq V_{\bar{n}(n)}^m(\vec{P}(\vec{A}_n) - \vec{f}_{\bar{n}(n)}) + V_{\bar{n}(n)}^m(\vec{f}_{\bar{n}(n)} - \vec{f}_{\bar{n}(n)}). \end{aligned}$$

Since  $\vec{A}_n$  solves (41), we see that the right side of the obtained

inequality is less than or equal to

$$\begin{aligned}
 & V_{\tilde{n}(n)}^m(\vec{P}(\tilde{A}_n) - \vec{f}_{\tilde{n}(n)}) + V_{\tilde{n}(n)}^m(\vec{f}_{\tilde{n}(n)} - \tilde{f}_{\tilde{n}(n)}) \\
 & \leq V_{\tilde{n}(n)}^m(\vec{P}(\tilde{A}_n) - \tilde{f}_{\tilde{n}(n)}) + 2V_{\tilde{n}(n)}^m(\vec{f}_{\tilde{n}(n)} - \tilde{f}_{\tilde{n}(n)}) \\
 & \leq \sqrt[m]{\tilde{n}(n)} \max_{l=1, n} |P(w_l, \tilde{A}_n) - f(w_l)| + 2V_{\tilde{n}(n)}^m(\vec{f}_{\tilde{n}(n)} - \tilde{f}_{\tilde{n}(n)}) \\
 & = \sqrt[m]{\tilde{n}(n)} \max_{l=1, n} \left| \sum_{k=n+1}^{\infty} a_k w_l^k \right| + 2V_{\tilde{n}(n)}^m(\vec{f}_{\tilde{n}(n)} - \tilde{f}_{\tilde{n}(n)}) \\
 & \leq \sqrt[m]{\tilde{n}(n)} \sum_{k=n+1}^{\infty} d_k r^k + 2V_{\tilde{n}(n)}^m(\vec{f}_{\tilde{n}(n)} - \tilde{f}_{\tilde{n}(n)})
 \end{aligned}$$

The right side of this inequality tends to zero when  $n$  goes to infinity. Thus we see that the polynomials  $P(w, \hat{A}_n)$  converge to  $f(w)$  at the points  $w_l, l = 1, 2, \dots$

Let us show that the sequence of polynomials  $P(w, \hat{A}_n)$  is bounded inside the disk  $K$ . Let  $0 < \rho < 1$  and  $|w| < \rho$ . Then we have

$$|P(w, \hat{A}_n)| \leq \sum_{k=0}^n d_k \rho^k \leq \sum_{k=0}^{\infty} d_k \rho^k.$$

The result now follows from the Vitali theorem, see [9]. □

**Acknowledgments.** The author is grateful to J.P. Prates Ramalho for helpful discussions of the problem and bibliographical support.

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