

***Избрани теми от Биоматематиката – примерна тема  
за изследователски проект (магистърска степен)***

По-долу предлагаме, като първоначален образец на тема за самостоятелно проучване (в рамките на магистърска програма), едно изследване, илюстриращо основните елементи в т.н. подход на Гибс – за математическо моделиране на състояния в хетерогенни материални системи.

**THE GIBBS APPROACH TO DIAGNOSTIC BIOMATHEMATICS.**

T. Boev, Pl. Georgiev<sup>1)</sup>, E. Molle<sup>2)</sup>

Department of Differential Equations, University of Sofia, 5 J. Boucher Ave., Sofia,  
Bulgaria

<sup>1)</sup>Department of Cell Biology, University of Sofia, 8 D. Tzankov Ave., Sofia, Bulgaria

<sup>2)</sup>Department of Genetics, University of Sofia, 8 D. Tzankov Ave., Sofia, Bulgaria

Corresponding author: [boev@fmi.uni-sofia.bg](mailto:boev@fmi.uni-sofia.bg)

**Abstract** A specified version of the classical Gibbs approach (for the so-called idealized description) is applied to get a mathematical model for the surface electrostatics of alveolus capillary vessels, in the human circulatory system, as a case of heterogeneous media. The found explicit formula for the electric potential relates to diagnostic methods in analyzing vessel-anomalies. It is solved a space-boundary transmission problem of an unconventional type, in spite of the equivalent surface phases surrounding a defect-line for a capillary. The potential-formula is established under the more general assumptions for existence of asymptotic surface power and nonlinear potential-dependence to the electric charges at the anomaly-contour.

**1. Introduction.**

A large segment of the natural sciences have been intensively engaged, since most of twenty years, to surface phenomena problems and the electrostatic properties of matter have been taken as the basic framework in the investigations. Two main directions of the said topics concern the surface nucleation phenomena in gas-liquid systems (see e.g. [16], [18], [2], [20]) – as a first example, and – as a second – the structure of semi conducting films of air-crystal media, via the technological interest to the films-growth and roughness (e.g. [14], [9], [6], [19]). After the important results in [1], the electrostatic viewpoint of heterogeneous material systems has been applied in most of the investigations. Note, as a next extension of the field, the recent studies on cell biology problems ([5]). By a precision of the tools in [2], a generalized method, based on the Gibbs ([8]) idealizing treatment, has been lately discussed ([17]) in cases of more complex heterogeneity. This is the case when the system is considered as a material composition of distinct bulk (3D), surface (2D) and line (1D) phases, under a model, estimated as enough adequate to the real phenomena. The contemporary problem now is centered in detecting the surface values of the electric potential.

We shall follow here the method from [17] to an air-air 3D material system (see Fig.1, below), with a flat (2D) organic interface, known as *lamina basalis*, cleft in two sub-phases by a (straight) line of functionally anomalous intercellular spaces (holes). The said construction is introduced as an admissible version of the real situation: a 3D localization is made to a capillary (practically cylindrical) vessel in the human white liver and the vessel-wall is (functionally) identified with its middle layer (the said lamina basale). Certain anomalies, in the air transfer, are presumably located on a curved (circular) line segment of lamina, across to the vessel-axis. Stretching (locally) the curved anomaly-line (and the surrounding cylindrical surface, together), we get the above-posed (flat-interfaced) construction. (We refer for the used notions e.g. to [13].) The presence of two-side bulk air phases is due to the anomalous air transfer: the outgoing stage gets blocked, after a previous air invasion. (See Sect. 2, for some additional phenomena-comments.)

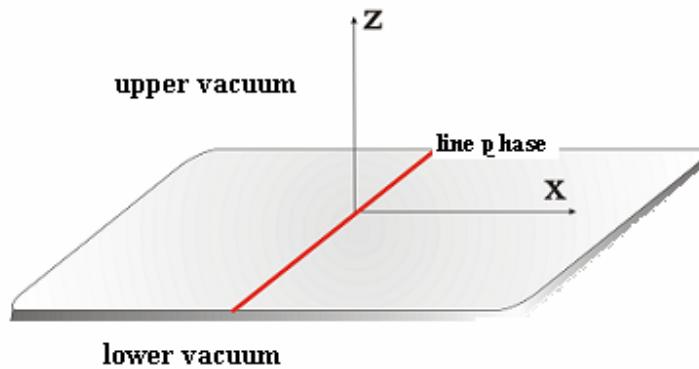


Fig. 1

This way we have given a typical case of 3-2-1 D heterogeneity, schematically shown on Fig. 1, above. The organic lamina-film is presented as the plain  $z=0$  (regarding a Cartesian  $(x,y,z)$ - coordinate system). A surface set of points (intercellular functional holes), with defective air permeability, is shaped a specific straight-line contour (the  $Oy$  - axis, Fig. 1). It separates the surface film into electrostatic equivalent halves – 2D material phases and plays, by a functional necessity, the role of an autonomous and materially homogeneous 1D phase. The air bulk phases will be treated as homogeneous and of vacuum; they fill respectively the upper semi-space,  $z > 0$  - the external to the capillary air medium, and - the lower one,  $z < 0$  - the internally blocked air. Thus the considered heterogeneous system includes upper and lower 3D vacuum sub-phases and a complex-structured organic interface (with a special role of a line phase).

We shall seek an explicit expression primarily for the interface electric potential of the system (as noted, it is the key factor in the electrostatics of complexly heterogeneous media). In the present study we follow the above-mentioned specified way, due to Radoev (e.g. [17]) - for mathematical modeling of electrostatics to the said type of heterogeneous media. The method introduces an extension of the Gibbs ([8])

idealizing approach and the Bedeoux-Vlieger ([2]) singular formalization of step transitions. For a short illustration to the method-essence, suppose given a material system of two near-by bulk phases  $B^-, B^+$ , with a common surface boundary  $S$ , consisting, as a material carrier, in two distinct 2D-phases,  $S^-, S^+$ . Additionally, the 2D (sub-) phases are separated by a line  $l$  – as a 1D material carrier, assumed homogeneous. From the viewpoint of a general modeling procedure, two basic tools have to be applied: the Maxwell electrostatic system, as a constituting-phenomena low - for the whole  $\{B^- \cup S \cup B^+\}$ - medium; two (or several) heterogeneity stages for introduction of material electrostatic characteristics:

$$(1.1) \quad G = G^- \eta^- + G^+ \eta^+ + G_s \delta_s;$$

$$(1.2) \quad G_s = G_s^- \eta_s^- + G_s^+ \eta_s^+ + G_l \delta_l.$$

Above  $G$  is a total electrostatic characteristic, distributed on the whole 3D medium. It is uniquely determined, under the singular decompositions (1.1), (1.2), by an ordered set of quantities,  $(G_l; G_s^\pm; G^\pm)$ . These quantities are supposed quasi-constants – i.e. constants or asymptotically constants and present the values of  $G$  on the sub-phases, of different sub-spaces and dimensions. In particular,  $G_s$  introduces the values of  $G$  on the surface  $S$ , by its singular decomposers  $G_s^\pm$ , characterizing respectively the surface sub-phases  $S^\pm$ . The 1D phase  $l$ , supposed homogeneous, is materially endowed by the quantity  $G_l$ . In (1.1)  $\eta^+$  ( $\eta^-$ ) is the (Heaviside) characteristic function for  $B^+$  ( $B^-$ ) and  $\delta_s$  is the Dirac delta-function, supported on the surface  $S$ . Next, by analogy, in (1.2)  $\eta_s^+$  ( $\eta_s^-$ ) is the characteristic function (defined on  $S$ ) for the semi-surface  $S^+$  ( $S^-$ ) and  $\delta_l$  is the Dirac delta-function, supported on  $l$ .

On Fig.1  $S$  is the plain  $z=0$ ;  $l$  is a straight line (the  $Oy$  axis). The air – air system is homogeneous however on the  $y$ -direction (because of the assumed homogeneity of the anomaly-line) and the electric potential  $u=u(x, y, z)$  depends consequently on  $x, z$  only, i.e.  $u=u(x, z)$ .

Applying systematically the above double-leveled scheme ((1.1)-(1.2)) in reworking of the Maxwell system (see Sect. 2), we establish the following final formulation to the sought mathematical model:

$$(1.3) \quad \nabla^2 u = 0 \ (z \neq 0), \ x \in R^1;$$

$$(1.4) \quad |u| \leq \text{const.}, \ (x, z) \in R^2;$$

$$\text{a)} \quad u(x, +0) = u(x, -0), \ x \in R^1;$$

(1.5)

$$\text{b)} \quad \varepsilon_b^+ u_z(x, +0) - \varepsilon_b^- u_z(x, -0) + \varepsilon_s u_{xx} = \varepsilon_s k_s^2 (u - \varphi_\infty), \ x \neq 0;$$

$$(1.6) \quad u(-\infty, 0) = \varphi_\infty^-, \ u(+\infty, 0) = \varphi_\infty^+;$$

$$\text{a)} \quad u(-0, 0) = u(+0, 0);$$

(1.7)

$$\text{b)} \quad \varepsilon_s^+ u_x(+0, 0) - \varepsilon_s^- u_x(-0, 0) = -\beta_l[u].$$

In (1.3)  $\nabla^2 \equiv \partial_x^2 + \partial_z^2$  is the La Place operator;  $u_x, u_z, u_{xx}$  are first or second order derivatives regarding the relevant variable;  $u(x, +0), u(x, -0)$  are respectively the limits (supposed finite)  $\lim_{z \rightarrow 0} u(x, z)$  (at  $z > 0$  or  $z < 0$ ), and, by analogy – for  $u_z(x, +0), u_z(x, -0); u(\pm 0, 0) = \lim_{x \rightarrow 0} u(x, 0)$  and  $u_x(\pm 0, 0) = \lim_{x \rightarrow 0} u_x(x, 0)$ , respectively at  $x > 0, x < 0$ , both – for  $u(\pm 0, 0)$  and  $u_x(\pm 0, 0); u(\pm\infty, 0) = \lim_{x \rightarrow \pm\infty} u(x, 0)$ . Parameters  $\varepsilon_b$  and  $k_s, \varepsilon_s$  are the main factors of the system-electrostatic nature; they are given step constants:  $\varepsilon_b = \varepsilon_b^+(z > 0), \varepsilon_b^- = \varepsilon_b^-(z < 0), \varepsilon_b^+, \varepsilon_b^-$  – positive (and different – in the more general situations);  $k_s = k_s^+(x > 0), k_s^- = k_s^-(x < 0)$  – in (1.5), with positive  $k_s^+, k_s^-$ ; by analogy,  $\varepsilon_s = \varepsilon_s^+(x > 0), \varepsilon_s^- = \varepsilon_s^-(x < 0)$  – in (1.5), (1.7), with  $\varepsilon_s^+ > 0, \varepsilon_s^- > 0$  – constants. The material meaning of parameter  $k_s$  is expressed by the quantity  $k_s^{-1} = \frac{1}{k_s}$ , known as the surface Debye length (e.g. [17]). Parameters  $\varepsilon_b, \varepsilon_s$  are respectively the bulk and surface dielectric permitivities, with  $\varepsilon_b^+(\varepsilon_b^-), \varepsilon_s^+(\varepsilon_s^-)$  – for the relevant bulk and surface phases. The asymptotic values of the potential are prescribed by the parameter  $\varphi_\infty$  (a given quantity):  $\varphi_\infty = \varphi_\infty^\pm$  (at  $x > 0, x < 0$ ), where  $\varphi_\infty^+, \varphi_\infty^-$  are real, generally different constants; the parameter  $\beta_l = \beta_l[u]$  enters as  $\beta_l = \frac{\rho_l}{\varepsilon_0}$  by  $\rho_l = \rho_l[u]$  – the density of the electric charges (supposed depending on potential  $u$ , Sect. 2) upon the line phase;  $\varepsilon_0 = 8.85 \text{ pF/m}$  is the so-called absolute dielectric permitivity. (Above  $R^m$  is the real  $m$  – dimensional Euclidean space,  $m = 1, 2, \dots$ )

In the equations (1.3) – (1.7), it is given a surface-line boundary problem of (new variant) transmission type – for the La Place equation (see (1.3)), regarding potential  $u$ . As already noted (e.g. in [3]), the essential differences, with the conventional one (cf. e.g. [4]), consist in the two, 2D and 1D (reduced actually to 1D and 0D – from the  $y$ -symmetry), interface conditions, including a second order differential term (see (1.5), (1.7)). The linear inclusion of  $u$  (in (1.3) and the term with  $\varepsilon_s k_s^2 u$ ) follows by taking the linear approximations (assumed adequate, see Sect. 2) of the relevant expressions for the bulk and surface charge density. By arguments of phenomenology, potential  $u$  will be searched for a bounded function (condition (1.4)), continuous in  $R^3$ , classically regular in the sets  $z \neq 0$  and  $x \neq 0 (z = 0)$ , with continuous gradients  $u_z, u_x$ , respectively at  $z \geq 0, z \leq 0$  (for  $u_z$ ), and  $x \neq 0 (z = 0)$  – for  $u_x$ . Summarizing the said requirements (for the potential), as a definition, the noted class of functions, satisfying the additional property  $u(x, 0) - \varphi_\infty \in L_2$  and relations (1.3) – (1.7) shall be called classical solutions to the problem (with  $L_2$  – the space of the squared-integrable functions).

The problem (1.3)–(1.7) shall be solved, assuming (as already noted) the upper and lower air phases ( $z > 0, z < 0$ ) as identical with vacuum; i.e. we have the assumption:

$$(1.8) \quad \varepsilon_b^- = \varepsilon_b^+ = 1.$$

As known, the key device in solving (1.3)-(1.7), this is the preliminary determination (by an explicit formula) of the surface potential. (Recall that such a solution formula is known from [17] and applied later in [19], but at the simpler case of  $\varphi_\infty^+ = \varphi_\infty^-$ .)

In Sect. 2 we begin with short comments on the phenomenology to the real surface structure of a single alveolar capillary vessel, as a special element in the human circulatory system, via the physiological necessity of the oxygen transfer. Next it is sketch the derivation of mathematical model (1.3)-(1.7). In Sect. 3 a basic presentation is found, for the surface potential and the related explicit formula is shown in case of charge parameter  $\beta_l$ , independent on potential, and assumed as a prescribed constant. In Sect. 4, as concluding remarks, two simple, but essential, cases of the non-linearity  $\beta_l[u]$  are shortly discussed regarding the solvability problem and a modified solution-formula is obtained, for the potential. Note the new moment here (in a comparison with [17]) coming from the nonlinear boundary condition (1.7.b).

## 2. Elements of phenomenology and mathematical modeling.

The general situation shows, in various samples of real heterogeneous matters (gas-liquid, in particular – gas-organic plasma, or air-solids), the so-called interfaces as actually bulk, but nanometers-scaled, transition zones (in particular, vessel-walls), treated as material 2D formations.

The interest of tools for biomedical detections of anomalies in the human circulatory system, via the walls-structure of the blood vessels, is directly motivated from the quite specific ruling function of the wall-layers. To recall and clarify the main (simplified) viewpoints here (cf. e.g. [13]), we assume a stretched location of the wall, as the flat surface ( $z = 0$ ) on Fig. 1. In reality this is a 3D organic threefold layer, deep not less than 120-180 nm. In our model we identify this layer with its middle part, of corpulence about 40-60 nm - it is just the so-called lamina basale (midmost) sub-layer - neglecting the upper (external) and lower (internal) ones. The neglected (internal and external) wall-layers, built respectively of endothelial and adventitiale cells, as a short description, are considered with a secondary role (compared to lamina basale). As known, acting as a typical bio-membrane, lamina basale is the main factor for the oxygen transfer to the blood. It is a polysacharide-matter, of fine fibers structure. Via the Gibbs approach (and taking into account the ratio of the wall corpulence to the radius of the capillary vessel, which is  $\ll 1$ ), we consider lamina basale layer as infinitely thin; thus we get an interface film of lamina basale matter (see the plain  $z = 0$  on Fig. 1) in an air-blood (vacuum-blood) heterogeneous 3D media. On the said 2D lamina film it is (uniformly) distributed a set of points – presenting the holes (tunnels, in reality radial to the vessel axis and known as intercellular spaces), which provide the oxygen contact to the blood; they are assumed however of certain functional anomaly, extremely activated on a relatively narrow strip (interpreted as a straight-line - the  $Oy$ -axis, Fig. 1). Thus an air volume left involved between the blood and the surface, shaping an internal (lower, on Fig. 2) air bulk phase; moreover, a specific 1D phase (of the extreme anomaly) is appeared ( $Oy$ -axis, Fig. 1). Interpreting the air zones as vacuum ones, we get that way the final constriction of the complex heterogeneous system under consideration (Fig. 1). The system consists in upper and lower vacuum bulk phases and a lamina-interface (as a 2D film). The interface structure includes two distinct (2D) halves; denote them by  $P^-, P^+$  (see the semi-planes  $x < 0$  ( $z = 0$ ) and  $x > 0$  ( $z = 0$ ) on Fig. 1 above). They are

treated, according to Gibbs, as materially (electrostatic) equivalent, but of different (electrostatic) nature, compared with the straight-line phase  $l$  ( $l = Oy$ , Fig. 1). To forecast certain influence of neighbouring vessel-zones, surface sub-phases  $P^-, P^+$  are presumed with prescribed values  $(\varphi_-, \varphi_+)$  of the electric potential, far from the phase contour  $l$ .

The next stage of this section is to sketch the basic step of modeling. Via the introduced framework (see Sect. 1) the key tool for description of electrostatic phenomena in complex media relates to the Maxwell system (in case of dielectrics, e.g. [15], [12]):

$$(2.1) \quad \text{a) } \nabla \cdot \mathbf{D} = \rho; \text{ b) } \mathbf{D} = -\epsilon_0 \epsilon \nabla u.$$

Here  $\nabla$  is the nabla operator,  $\mathbf{D}$  is the vector of the electric induction ([15]), called also (in Electrochemistry, e.g. [11]) electric displacement,  $\nabla \cdot \mathbf{D}$  is the formal scalar product of the vectors nabla and  $\mathbf{D}$ , i.e.  $\nabla \cdot \mathbf{D} = \operatorname{div} \mathbf{D}$ ;  $\rho$  is the charge density;  $\epsilon$  is the relative dielectric permittivity for the relevant part of the medium (in particular  $\epsilon = \epsilon_b^-$ , at  $z < 0$ ,  $\epsilon = \epsilon_s$ , at  $z = 0, x \neq 0$ );  $u$  is the electric potential,  $\nabla u = \operatorname{grad}(u)$ , where  $(-\nabla u)$  represents the electric field, propagated in the whole 3D material system. Equations (2.1) hold for the total (3D) system and, as known, potential  $u$  is a continuous function of  $(x, y, z)$ , in spite of the various material phases; the heterogeneity of the system is indicated however mainly by the quantities  $\mathbf{D}$  and  $\rho$  (note that the permittivity  $\epsilon$  enters in these quantities). Next, from the singular decomposition principle (Sect. 1, (1.1)-(1.2)), applied now for  $G = \mathbf{D}$  and  $G = \rho$ , we come to the following problem. Find the (admissibly regular) solutions  $(\mathbf{D}, u)$  to (2.1), corresponding to the said singular decompositions.

*Remark:* Equation (2.1.b) is realized as equivalent to the system

$$\{\mathbf{D} = -\epsilon_0 \epsilon \nabla u \ (z \neq 0), \vec{D}_s^\tau = -\epsilon_0 \epsilon_s \partial_x^2(u_s) \ (z = 0, x \neq 0), \vec{D}_l^\tau = \vec{0} \ (z = 0, x = 0)\}.$$

Here  $\vec{D}_s^\tau, \vec{D}_l^\tau$  are the tangential, respectively to the plain  $z = 0$  and the contour  $l$ , components of these vectors, denoted by  $\mathbf{D}_s, \mathbf{D}_l$ , which represent the field  $\mathbf{D}$  via the singular decompositions (1.1)-(1.2);  $u_s = u(z = 0)$ . We have taken into account the symmetry on the  $y$ -direction, i.e.  $u = u(x, z)$ .

Now, combining the Maxwell electrostatic laws and the two-leveled decomposition scheme, we find, as an initial version of the needed model, the following system regarding the basic quantities (the various bulk, surface and line phases enters then clearly distinguished):

$$(2.2.a) \quad \nabla \cdot (\mathbf{D}_b)^+ = \rho_b^+ \ (z > 0), \nabla \cdot (\mathbf{D}_b)^- = \rho_b^- \ (z < 0);$$

$$(2.2.b) \quad (\mathbf{D}_b)^+ = -\epsilon_0 \epsilon_b^+ \nabla u \ (z > 0), (\mathbf{D}_b)^- = -\epsilon_0 \epsilon_b^- \nabla u \ (z < 0);$$

$$(2.3.a) \quad D_+^\varepsilon(x, 0) - D_-^\varepsilon(x, 0) + \nabla_s \cdot \mathbf{D}_s = \rho_s \ (z = 0, x \neq 0);$$

$$(2.3.b) \quad \mathbf{D}_s = -\epsilon_0 \epsilon_s \cdot \nabla_s u_s \quad (z=0, x \neq 0);$$

$$(2.4) \quad \bar{D}_s^{x,+} - \bar{D}_s^{x,-} = \rho_l.$$

Above we have applied decompositions (1.1), (1.2) in several specified cases:

$$\begin{aligned} \rho &= \rho_b^- \eta^-(z) + \rho_b^+ \eta^+(z) + \rho_s \delta(z); \quad \rho_s = \rho_s^- \eta_s^- + \rho_s^+ \eta_s^+ + \rho_l \delta_l; \\ \mathbf{D} &= (\mathbf{D}_b)^- \eta^-(z) + (\mathbf{D}_b)^+ \eta^+(z) + \mathbf{D}_s \delta(z). \end{aligned}$$

Here  $\eta^+(z)/\eta^-(z)$  are respectively the Heaviside forward/backward functions (i.e.  $\eta^+(z)=1$ , at  $z>0$ ,  $\eta^+(z)=0$ , at  $z<0$ ,  $\eta^-(z)\equiv\eta^+(-z)$ ) and  $\delta(z)$  is the Dirac delta-function, supported at  $z=0$ ;  $\eta_s^- = 1$ , at  $z=0, x<0$  and  $\eta_s^- = 0$ , at  $z=0, x>0$ , by analogy:  $\eta_s^+ = 1$ , at  $z=0, x>0$  and  $\eta_s^+ = 0$ , at  $z=0, x<0$ ; next,  $\delta_l$  is delta-function, supported on the line  $l: x=0$ , and we shall also use the notation  $\delta(x)$ , for  $\delta_l$ ;  $\nabla_s$  is the tangential (to  $z=0$ ) component of the nabla operator  $\nabla$  and  $\bar{D}_s^{x,+}, \bar{D}_s^{x,-}$  are the relevant limits (assumed finite), at  $x \neq 0$ , for the normal to  $l$  component  $\bar{D}_s^x$  of  $\mathbf{D}_s$ . (Note that the used derivations of the Heaviside and Dirac delta-functions are taken in the Schwartz distributions meaning, e.g. [21], [10].)

Next, let us comment the charge density term  $\rho$  in (2.1). It should be noted here that  $\rho$  depends on the space variables by the potential  $u$ , i.e.  $\rho = \rho[u]$ . The said dependence is well known for electrolytes by the Gouy-Chapmann theory, where  $\rho[u]$  is expressed by the so-called Boltzmann distribution (see e.g. [11]). In case of vacuum it holds the relation  $\rho[u] = o(u) (|u| \ll 1)$  and for the linear approximations  $\rho_{b,L}^-[u], \rho_{b,L}^+[u]$ , respectively of  $\rho_b^-[u], \rho_b^+[u]$  we shall have  $\rho_{b,L}^-[u] = \rho_{b,L}^+[u] = 0$ . Now we are going to take in (2.2)-(2.4) the linear approximations of  $\rho_b^\pm, \rho_s$  instead. A preliminary motivation to do that follows from the argument that the polysaharidean matter of the interface admits to consider it as a lipid medium, where the potential-magnitude can be assumed relatively smaller than the basic ratio  $(RT_0)/F$ , which yields that linear approximations become acceptable ( $F, R, T_0$  are – as follows – the so-called Faraday and gas constants, and the absolute temperature). The Boltzmann principle, applied for surfaces, suggests (e.g. [17]) dependences  $\rho_s^\pm = \rho_s^\pm[u - \varphi_\infty]$ , to the surface phases, with  $\rho_{s,L}^\pm[u - \varphi_\infty] = -\epsilon_0(k_s^\pm)^2 \cdot (u_s - \varphi_\infty)$ , for the linear approximations. On the linear (1D) phase, the contour  $l = Oy$ , we prefer however a nonlinear Boltzmann type model  $\rho_l = \rho_l[u]$ , forecasting possible unknown complications, close to the line contour.

Then the second basic step of modeling is to introduce the above-commented (linear) approximation. Inserting the relevant approximants instead, in (2.2)-(2.4), we get:

$$(2.5.a) \quad \nabla \cdot (\mathbf{D}_b)^+ = 0 \quad (z > 0), \quad \nabla \cdot (\mathbf{D}_b)^- = 0 \quad (z < 0);$$

$$(2.5.b) \quad (\mathbf{D}_b)^+ = -\epsilon_0 \nabla u \quad (z > 0), \quad (\mathbf{D}_b)^- = -\epsilon_0 \nabla u \quad (z < 0);$$

$$(2.6.a) \quad D_+^z - D_-^z + \nabla_s \cdot \mathbf{D}_s = -\epsilon_0 \epsilon_s k_s^2 (u_s - \varphi_\infty) \quad (z=0, x \neq 0);$$

$$(2.6.b) \quad \mathbf{D}_s = -\epsilon_0 \epsilon_s \nabla_s u_s \quad (z=0, x \neq 0);$$

$$(2.7) \quad \vec{D}_s^{x,+} - \vec{D}_s^{x,-} = \rho_l[u].$$

In the right hand sides of the equations in (2.5.a) we have taken into account the vacuum-conditions (except the electro-neutrality-hypothesis for the total 3D medium).

Finally, it remains to apply a slight reworking on the above-posed, (2.5)-(2.7) – stage, of the model We shall firstly express  $(\mathbf{D}_b)^+$ ,  $(\mathbf{D}_b)^-$  in (2.5.a) by the right hand sides from (2.5.b) and come this way to the La Place equations from (1.3). (Note that condition (1.4) corresponds to the physical nature of the potential – to be a bounded and continuous function of  $(x, y, z)$ .) Looking to the next relations in the problem (1.3)-(1.7), the included-ones in (1.5.a), (1.7.a) show that potential stays continuous across the transition surfaces and lines. On the other hand condition (1.6) introduces the asymptotic value of the surface potential  $u_s$  - they are considered as experimentally known (gauged) data. Secondly, we replace  $\mathbf{D}_s$  in (2.6.a) by the right hand side of (2.6.b) and use that  $D_+^z(x, 0) = -\epsilon_0 \epsilon_b^+ u_z(x, +0)$ ,  $D_-^z(x, 0) = -\epsilon_0 \epsilon_b^- u_z(x, -0)$ , with  $\epsilon_b^\pm = 1$ . Thus we get, from (2.6), the specific jump condition (1.5.b). Concerning the second jump-condition for the electric field (see (1.7.b)), recall that  $\rho_l = \epsilon_0 \beta_l$  and  $\vec{D}_s^{x,\pm} = -\epsilon_0 \epsilon_s u_x(\pm 0, 0)$ .

Thus the derivation of the final variant (1.3) – (1.7), posed in Sect. 1, is completed and the sought mathematical model is presented as a two-leveled (surface-line) transmission problem.

### 3. Explicit expressions to the surface electric potential.

Our main goal here will be to find presentations of an explicit type, for the surface values  $u(x, 0)$  of the electric potential and a final formula in the linear case of the charge density  $\rho_l$ , i.e.  $\beta_l[t] \equiv const.$ . We shall use the  $x$ -Fourier transformation of potential  $u(x, z)$ .

If  $u = u(x, z)$  is a classical solution to problem (1.3) – (1.7), let us denote by  $\hat{u}(\xi, z)$  the (partial) Fourier transformation of  $u(x, z)$  - with respect to  $x$ , where  $\xi$  is the dual to  $x$  variable. The following conventional expressions shall be taken into account:

$$(3.1) \quad \hat{\Phi}(\xi) = \int \Phi(x) \exp(-ix\xi) dx; \quad \Phi(x) = \frac{1}{2\pi} \int \hat{\Phi}(\xi) \exp(ix\xi) d\xi.$$

In (3.1)  $\Phi$  is supposed (for the sake of simplicity) in the Schwartz class of the fast decreasing functions (e.g. [10]) and the integrations are taken from  $-\infty$  to  $+\infty$ . Applying the  $x$ -Fourier transformation to the relations in (1.3), we find ordinary differential equations (regarding  $z$ ), which, because of (1.4), yield for  $\hat{u}(\xi, z)$  the known presentations:

$$(3.2) \quad \hat{u}(\xi, z) = \hat{\phi}(\xi) \exp(-|z||\xi|), z \neq 0.$$

Above  $\varphi(x) = u(x, 0)$  and  $\hat{\varphi}$  is the Fourier map of  $\varphi$ . The jump term in (1.5.b) can be then expressed by the following way:

$$(3.3) \quad \begin{aligned} u_z(x, +0) - u_z(x, -0) &= L[\varphi], \\ (L[\varphi])\hat{(\xi)} &\equiv -2|\xi| \hat{\varphi}(\xi). \end{aligned}$$

It is clear that in (3.3) it is given a linear operator  $L: \varphi \rightarrow L[\varphi]$ , acting from  $L_2(R^1)$  into the Sobolev space  $H^{-1}(R^1)$  (we refer e.g. to [10], for the  $H^k$ -spaces of Sobolev). With the said operator the system (1.3) – (1.7) is splitting in two separate types of problems:

*The Dirichlet problems –*

$$(3.4.a) \quad \nabla^2 u = 0 \quad (z \neq 0);$$

$$(3.4.b) \quad u(x, 0) = \varphi(x), \quad x \in (-\infty, +\infty);$$

*The boundary transmission problem –*

$$(3.5.a) \quad L[\varphi] + \varepsilon_s \varphi'' = \varepsilon_s k_s^2 (\varphi - \varphi_\infty), \quad z = 0, x \neq 0;$$

$$(3.5.b) \quad \varphi(\pm\infty) = \varphi_\infty^\pm, \quad \varphi(+0) = \varphi(-0);$$

$$(3.5.c) \quad \varepsilon_s [\varphi'(+0) - \varphi'(-0)] = -\beta_l[\varphi].$$

We have used the notations  $\varphi'$  and  $\varphi''$  respectively for the first and second derivative of  $\varphi(x)$  and  $\varphi(\pm\infty)$ ,  $\varphi(+0)$ ,  $\varphi(-0)$ ,  $\varphi'(+0)$ ,  $\varphi'(-0)$  – for the relevant limits. By the substitution  $\psi(x) \equiv \varphi(x) - \varphi_\infty$  we shall reduce the problem (3.5) into a simpler one. Let us firstly calculate the quantity  $L[\varphi]$  by  $L[\psi]$ ; if set  $\sigma[\varphi_\infty] = \varphi_\infty^+ + \varphi_\infty^-$  and  $\Delta\varphi_\infty = \varphi_\infty^+ - \varphi_\infty^-$ , we get  $L[\varphi] = L[\psi] + \frac{1}{2}(\sigma[\varphi_\infty]L[1] + \Delta\varphi_\infty L[sg])$ , where  $sg$  is the known sign - function,  $sg(x) = \frac{x}{|x|}$ . It is directly seen that  $L[sg](x) = 2\sigma_0(x)$ , where  $\sigma_0(x) : \hat{\sigma}_0(\xi) = i.sg(\xi)$  ( $i = \sqrt{-1}$ ), and  $L[1] = 0$ . Then, from (3.5), we go to the next reduced problem for  $\psi$ :

$$(3.6) \quad \psi'' - k_s^2 \psi = -\frac{1}{\varepsilon_s} (L[\psi] + \Delta\varphi_\infty \cdot \sigma_0), \quad x \neq 0;$$

$$(3.7) \quad \varepsilon_s [\psi'(+0) - \psi'(-0)] = -\beta_l[\varphi].$$

The simplified  $\psi$ -problem ((3.6)-(3.7)) is presumably considered in the space of the real functions which are continuous in  $(-\infty, -0]$ ,  $[+0, +\infty)$ , tend to zero, at  $|x| \rightarrow \infty$  and belong to  $L_2(R^1)$ ; in addition they are assumed to have the classical regularity at  $x \neq 0$ , with finite values of the limits  $\psi'(\pm 0)$ . Our next step is to transform the boundary problem (3.6)-(3.7) to an integral relation. To that goal, observe before that, with a given

solution  $\psi$  of (3.6) – from the said class, we actually have a regular enough, bounded solution to the equation

$$(3.8) \quad w'' - k_s^2 w = -\frac{1}{\varepsilon_s} (L[\psi] + \Delta\varphi_\infty \cdot \sigma_0), \quad x \neq 0.$$

Now let us introduce the following auxiliary functions, related, by the Fourier transformation, to the relevant components in the right hand side of (3.8):

$$(3.9) \quad g(x) = -\frac{1}{\pi} \int_0^\infty \frac{\sin(x\xi)}{k_s^2 + \xi^2} d\xi ;$$

$$(3.10) \quad w_s[\psi](x) = \frac{1}{2k_s} L[\psi]^* \exp(-k_s |x|)(x).$$

Above  $F^*\Phi$  is the convolution of two (Schwartz) distributions,  $F$  and  $\Phi$  (see e.g. [10]), and  $w_s[\psi]$  determine actually a bounded linear operator,  $w_s : L_2(R^1) \rightarrow H^1(R^1)$ .

Now it can be verified that function  $\frac{1}{\varepsilon_s} (w_s[\psi](x) + \Delta\varphi_\infty \cdot g(x))$  is a bounded partial solution to (3.8); therefore function  $\psi$  (the solution of (3.6)), as a solution of (3.8), from the said class, has to be in the form:

$$(3.11) \quad \psi(x) = c \exp(-k_s |x|) + \frac{1}{\varepsilon_s} (w_s[\psi](x) + \Delta\varphi_\infty \cdot g(x)), \quad x \neq 0.$$

Here  $c$  is a free step-constant,  $c = c^\pm (x \neq 0)$ . We have to identify this free parameter (by inserting from (3.11) in condition (3.7)). The right hand side of (3.11), rewritten shortly as  $\Phi_s(x)$  (where  $\Phi_s = \Phi_s[\psi]$ ) presents however a function in the class  $H^1(R^1)$  and, by equality  $\psi(x) = \Phi_s(x), x \neq 0$  (identical to (3.11)), it is seen that derivative  $\psi'$  (as a Schwartz distribution from the space  $H^{-1}(R^1)$ ) belongs both to  $L_2(-\infty, 0)$  and  $L_2(0, +\infty)$ . A direct calculation of  $\Phi'_s$  (in the sense of distributions) yields the relation  $\psi'(x) = \psi_1(x) + \Delta\psi(0) \cdot \delta(x)$ , with a function  $\psi_1 \in L_2(-\infty, +\infty)$  ( $\psi_1 = \Phi'_s$ , in the  $L_2(-\infty, +\infty)$  sense) and  $\Delta\psi(0) \equiv \psi(+0) - \psi(-0)$ ; i.e., for each solution  $\psi$  of (3.6) – of the mentioned class, with  $\Delta\psi(0) = -\Delta\varphi_\infty$ , it holds (in the sense of distributions):  $\psi'(x) = \psi_1(x) - \Delta\varphi_\infty \cdot \delta(x)$  (with  $\psi_1 \in L_2$ ),  $\delta(x)$  - the Dirac-function. Then, differentiating the expressions for  $g(x)$  and  $w_s[\psi]$  (see (3.9), (3.10)), we find respectively:

$$\begin{aligned} g'(x) &= w_s[\delta](x); \\ (w_s[\psi])'(x) &= w_s[\psi_1](x) - \Delta\varphi_\infty \cdot w_s[\delta](x); \\ \Delta\varphi_\infty \cdot g'(x) + (w_s[\psi])'(x) &= w_s[\psi_1](x). \end{aligned}$$

Above we have used that operator  $w_s$  acts also from  $H^{-1}(R^1)$  into  $L_2(R^1)$ , so that  $w_s[\delta](x) \in L_2(R^1)$ , and the expression of  $g'(x)$ . Consequently, derivative  $\psi'$  is presented by the formula:

$$(3.12) \quad \psi'(x) = -ck_s sg(x) \exp(-k_s |x|) + \frac{w_s[\psi_1](x)}{\varepsilon_s}, \quad x \neq 0.$$

Function  $w_s[\psi_1](x)$  is continuous on  $R^1$  (because  $\psi_1 \in L_2$ ) and, substituting by (3.12) in (3.7), we get  $\varepsilon_s k_s(c^+ + c^-) = \beta_l[\varphi]$ ; on the other hand, calculating the jump  $\Delta\psi(0)$  by (3.11), it holds the additional relation  $c^+ - c^- = -\Delta\varphi_\infty$ . Then, from the so-found elementary system for  $c^+, c^-$ , we obtain the unique value  $c = c_s$ , with

$$(3.13) \quad c_s = \frac{1}{2} \left( \frac{\beta_l}{\varepsilon_s k_s} - \Delta\varphi_\infty \cdot sg(x) \right).$$

Now, for the sake of convenience to the final formula let us introduce the function

$$(3.14). \quad \psi_s^0(x) \equiv \frac{1}{\pi} \int_0^\infty \frac{\cos(x\xi) d\xi}{2\xi + \varepsilon_s(k_s^2 + \xi^2)}.$$

Remark: The function from (3.14) determines, as *the canonical surface potential*, the solution of the (canonical) problem – (3.6)-(3.7), with  $\Delta\varphi_\infty = 0$ ,  $\beta_l \equiv 1$ .

Let us denote by  $\psi_s^{0,1}$  the first-order derivative of function  $\psi_s^0$  and apply the Fourier transformation to (3.11), with  $c = c_s$ . This yields the final expression of  $\psi$  and, by the substitution  $\varphi = \psi + \varphi_\infty$  - the sought basic formula:

$$(3.15) \quad \varphi(x) = \varphi_\infty + \beta_l[\varphi] \psi_s^0(x) + \varepsilon_s \Delta\varphi_\infty \cdot \psi_s^{0,1}(x) + \Delta\varphi_\infty \cdot g(x).$$

In the partial case  $\beta_l[u] \equiv \beta_l^0$  ( $\beta_l^0$  - constant), as a direct corollary it holds the following result.

**Proposition 1.** For each choice of the parameters  $\varepsilon_s > 0$ ,  $k_s > 0$ ,  $\varphi_\infty^\pm$ ,  $\beta_l^0$  (arbitrary constants) the problem (1.3)-(1.7) (at  $\beta_l = \beta_l^0$ ) possesses a unique classical solution  $u(x, z)$  with surface values  $u(x, 0) = \varphi(x)$ , determined by the formula

$$(3.16) \quad \varphi(x) = \varphi_\infty + \beta_l^0 \psi_s^0(x) + \Delta\varphi_\infty [\varepsilon_s \psi_s^{0,1}(x) + g(x)].$$

*The proof* has been actually already done – by the above said arguments (expression (3.15)) it follows that function  $\varphi(x)$  from (3.16) is the unique solution (with the assumed regularity and asymptotic values at  $|x| \rightarrow \infty$ ) of the boundary transmission problem (3.5), at data including constant  $\beta_l^0$ , instead of  $\beta_l[\varphi]$  in condition (3.5.c). Next the space potential  $u(x, z)$  is uniquely determined by the conventional Dirichlet problems (3.4) under the boundary condition  $u(x, 0) = \varphi(x)$  (for already given data  $\varphi(x)$ ). To

express explicitly potential  $u(x, z)$ ,  $\forall(x, z), z \neq 0$ , it remains to apply the well known (e.g. [22], [7]) semi-plane formula for the Dirichlet problem to the La Place equation.

#### 4. Concluding remarks – the nonlinear case in the second jump condition.

Here we shall analyze the solvability of the (surface) problem (3.5) with nonlinear charge-density function  $\beta_l[t]$ , in condition (3.5.c), assumed generally as a Boltzmann type distribution. The accent will be made on two basic cases for  $\beta_l[t]$  - either convex or concave, at  $t \geq 0$ . Without any loss of generality (via the finite sum of exponents in the Boltzmann distribution, e.g. [11]), function  $\beta_l[t]$  is supposed to have continuous derivatives up to second order,  $\forall t$ . It turns out a simple type relation has to be forecasted, between the values  $\beta_l[0]$  and  $\sigma[\varphi_\infty] = \varphi_\infty^- + \varphi_\infty^+$ . Let us introduce the next several assumptions:

$$(4.1.a) \quad \beta_l[+\infty] = +\infty, \beta_l''[t] > 0, t \geq 0;$$

$$(4.1.b) \quad \sigma[\varphi_\infty] < -2\psi_s^0(0) |\beta_l[0]|.$$

$$(4.2.a) \quad 0 < \beta_l[0] < \beta_l[+\infty] < +\infty, \beta_l''[t] < 0, t \geq 0;$$

$$(4.2.b) \quad -2\psi_s^0(0)\beta_l[0] < \sigma[\varphi_\infty].$$

$$(4.3.a) \quad \beta_l[0] \leq 0, \beta_l[+\infty] = +\infty, \beta_l''[t] > 0, t \geq 0;$$

$$(4.3.b) \quad 0 \leq \sigma[\varphi_\infty] < 2\psi_s^0(0) |\beta_l[0]|.$$

$$(4.4.a) \quad 0 < \beta_l[+\infty] < +\infty, \beta_l''[t] < 0, t \geq 0;$$

$$(4.4.b) \quad 2\psi_s^0(0) |\beta_l[0]| < \sigma[\varphi_\infty].$$

Recall that function  $\psi_s^0(x)$  is the given one by (3.14), where from it is seen  $\psi_s^0(0) > 0$ ; moreover this positive value can be easily calculated. On the other hand, for the left and right boundary values of the derivative  $\psi_s^{0,1}$  (at  $x = 0$ ), it will be not difficult to verify that  $\varepsilon_s \psi_s^{0,1}(-0) = \frac{1}{2}$  and  $\varepsilon_s \psi_s^{0,1}(+0) = -\frac{1}{2}$ . Now applying twice the basic presentation (3.15) at  $x = 0$  (under the preliminary observation for  $g(0) = 0$ ), we get:

$$\varphi(0) = \varphi_\infty^- + \beta_l[\varphi(0)]\psi_s^0(0) + \frac{\Delta\varphi_\infty}{2}; \quad \varphi(0) = \varphi_\infty^+ + \beta_l[\varphi(0)]\psi_s^0(0) - \frac{\Delta\varphi_\infty}{2}.$$

Then summing up (the above equalities), we find:

$$(4.5) \quad \varphi(0) - \frac{\sigma[\varphi_\infty]}{2} = \psi_s^0(0)\beta_l[\varphi(0)].$$

Consequently a possible value for the key potential of the line phase  $\varphi(0)$ , can be found solving, regarding  $t$ , the simple equation:

$$(4.6) \quad t - \frac{\sigma[\varphi_\infty]}{2} = \psi_s^0(0)\beta_l[t], \quad t \geq 0.$$

It will be enough however to use elementary geometric arguments. In the auxiliary  $(t, Y)$ -coordinate plane compare the straight line  $Y = \frac{1}{\psi_s^0(0)} \left( t - \frac{\sigma[\varphi_\infty]}{2} \right)$  with the curve  $Y = \beta_l[t]$ , at  $t \geq 0$ . It can be established, at each of cases (4.1)-(4.4), existence of a unique positive value  $t = \varphi^0$  determining the intersection point of the straight line and the said curve. Thus we come to the following conclusion.

**Proposition 2.** For each choice of parameters  $\varepsilon_s > 0, k_s > 0$  (arbitrary constants), function  $\beta_l[t]$  and parameters  $\varphi_\infty^\pm$ , satisfying some of conditions (4.1)-(4.4), the nonlinear surface (line) transmission problem (3.5) possesses a unique classical solution  $\varphi(x)$ , with a positive value  $\varphi(0) = \varphi^0$  - the root of the equation (4.6), given by the formula

$$(4.7) \quad \varphi(x) = \varphi_\infty + \left( \varphi^0 - \frac{\sigma[\varphi_\infty]}{2} \right) \frac{\psi_s^0(x)}{\psi_s^0(0)} + \Delta\varphi_\infty [\varepsilon_s \psi_s^{0,1}(x) + g(x)].$$

*The proof* follows now immediately from the above-mentioned arguments.

The above result completes an analysis to the more general case of contour charges (on the extreme anomaly line), depending nonlinearly on the electric potential.

**Acknowledgement.** The study is devoted to the 120-th anniversary of the Sofia University “St. Kliment Ohridski”.

It was partially supported by grant No 84/2007 of the Sofia University Science Foundation.

The authors are grateful to Dr. R. Slavchov (Dep. Phys. Chem., Sofia Univ.) for the assistance in preparing the illustration and to Assoc. Prof. L. Valkov (Tech. Univ. of Rousse (Bulg.)) – for the useful information on IMA Preprint Series.

## References

1. Bedeaux, D., Vlieger, J., A phenomenological theory of the dielectric properties of thin films, *Physica* **67** (1973) 55-73.
2. Bedeaux, D., Vlieger, J., *Optical Properties of Surfaces*, Imperial College Press, London(2001).

3. Boev, T., Radoev, B., Slavchev, R. Surface electrostatics of heterogeneous media. Mathematical models, problems and methods, Proc. of the 10thy Nat. Congress on TAM, 2005, Volume 1, 427 – 445.
4. Colton, D., Kress, R., Integral Equation Methods in Scattering Theory, John Wiley & Sons, New York (1983).
5. Cook, B., Kazakova, T., Madrid, P., Neal, J., Pauletti, M., Zhao, R., Cell-foreign Particle Interaction, IMA Preprint Series # 2133-3 (Sept. 2006), Univ. of Minnesota.
6. Ebert, Ph., Hun Chen, Heinrich, M., Simon, M., Urban, K., Lagally, M.G., Direct Determination of the Interaction between Vacancies on InP(110) Surfaces, Phys.Rev.Lett., **76**, (№ 12), 18 March 1996.
7. Genchev, T., Partial Differential Equations, Sofia Univ. Ed., Sofia (1999) (in Bulgarian).
8. Gibbs, J., The Scientific Papers, **1**, Dover, New York (1961).
9. Heinrich, M., Ebert, Ph., Simon, M., Urban, K., Lagally, M.G., Temperature Dependent Vacancy Concentrations on InP(110) Surfaces, J. Vac. Sci. Technol. A. **13**(3), May/Jun. 1995.
10. Hörmander, L., The Analysis of Linear Partial Differential Operators, v. I-IV, Springer-Verlag, Berlin (1983).
11. Israelishvili, J., Intermolecular and Surface Forces, Academic Press, London (1991).
12. Jackson, J.D., Classical Electrodynamics, John Wiley & Sons, New York, (1962).
13. Junqueira, Z., Carneiro, J., Kelly, R.O., Basic Histology, A. ZANCE Medical Book (1995).
14. Krčmar, M., Saslow, W., Weimar, M. Electrostatic Screening near Semiconductor Surfaces, Phys. Rev. B **61** (1999) 18321-18332.
15. Landau, L., Lifschitz, S., Lectures on Modern Physics, vol. VIII Electrodynamics of Solids, Nauka (Moscow) 1982 (in Russian).
16. Möhwald, H. Phospholipid and Phospholipid-Protein Monolayers at the Air/Water Interface, Annu. Rev. Phys.Chem., **41** (1990) 441-476.
17. Radoev, B., Boev, T., Avramov, M. Electrostatics of Heterogeneous Monolayers, Adv. In Colloid and Interface Sci., **114-115** (2005) 93-101.
18. Seul, M. Andelman D. Domain Shapes and Patterns of Modulated Phases, Science, **267** (1995) 476-483.
19. Slavchov, R., Ivanov, Tz., Radoev, B., Screened potential of a charged step defect on a semiconductor surface J. Phys.: Condens. Matter **19**(2007) 226005 (6pp).
20. Stoeckelhuber, K.W., Radoev, B., Wenger, A. and Schulze, H.J., Rupture of wetting films caused by nano-bubbles, Langmuir, 20 (2004), 164.
21. Schwartz, L., Theorie des Distributions, Herman, Paris (1950).
22. Tihonov, A., Samarskiy, A., Equations of Mathematical Physics, Nauka, Moscow (1972) (in Russian).