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Consistent Electrostatics of Crystalline Conductor: 4. Fully Consistent Phenomenological Model

by Michael Grinfeld and Steven Segletes

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The conductor model of Grinfeld et al.[2] permits the negatively charged boundary layers with finite 2-D magnitude (i.e., with infinite 3-D magnitude). Therefore, in this report we modify our model one more time to eliminate the appearance of negatively charged boundary layers with infinite 3-D magnitude. We do this along the lines of Grinfeld and Grinfeld (i.e., taking into account the thermodynamic internal energy density of charged negative liquid).

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Contents

1. Introduction

This report is a continuation of the series of studies and reports[1–3] aimed at the elimination of some inconsistences in the classical electrostatics. The main inconsistency, discussed in detail in Grinfeld and Segletes,[1] is reflected in the appearance of the surface layers of electric charge in the vicinity of the conductors' boundaries. Formally, these layers have the finite 2-D mass density. In fact, this means that the standard 3-D densities of the negative or positive charges have the magnitude equal to infinity. Obviously it is highly desirable to eliminate all these sort of paradoxical inconsistencies. They contradict standard experimental physics, which deals with fields or high magnitudes but never with the infinitely large fields. Also, this sort of modeling defect causes various difficulties in the numerical implementation and in the consistent modeling of novel effects.

The paradox of infinitely high density of charge is particularly striking in what concerns the positive charges at the boundaries of solid conductors. Basically, in all models of crystalline conductors, the densities of those positive charges are not only finite but also fixed. Therefore, in Grinfeld et al.[2] we first reformulated the classical electrostatics in such a way that no positively charged boundary layers with finite 2-D density can appear. We formulated the modified model in the form of the boundary value problem and illustrated our approach by considering the conducting slab. Later, Segletes[3] analyzed another instructive model dealing with a spherical conductor.

Still, the model of Grinfeld et al.[2,3] permits the negatively charged boundary layers with finite 2-D magnitude (i.e., with infinite 3-D magnitude). Therefore, in this report we modify our model one more time to eliminate the appearance of negatively charged boundary layers with infinite 3-D magnitude. We do this along the lines of Grinfeld and Grinfeld[4–6] (i.e., taking into account the thermodynamic internal energy density of charged negative liquid).

2. Formulation of the 1-D Boundary Value Problem (BVP)

We follow here the report of Grinfeldet al.[2] and Section 8 of Grinfeld and Grinfeld.[5] Per these reports, the entire system of equilibrium equations includes the following three elements:

1) The condition of thermal equilibrium

$$T = T^{\circ} = const \qquad (1)$$

throughout the whole configuration, where T is the absolute temperature.

2) The electrostatics system

$$\frac{d^2\varphi}{dz^2} = -4\pi\left(\sigma_e\rho_e + \sigma_i\rho_i\right) \tag{2}$$

where σ_e, σ_i are the respective charge densities per unit mass of the negative (mobile) charge and positive (immobile) charge components per unit mass, and ρ_e, ρ_i are the mass densities of the components; φ is the electric potential.

3) The electrochemistry equation for the mobile charges

$$\left(\rho e\right)_{\rho_e} + \sigma_e\varphi = \Lambda_e \tag{3}$$

where Λ_e is the indefinite Lagrange multiplier.

To determine the Lagrange multiplier, we have to use the equation dealing with the total charge (or mass) of the mobile negative charges. Let M_e be the total mass of the column of the mobile charges with a unit cross-section. This leads to the relationship

$$\int_{-H}^{H} dz\rho_e\left(z\right) = M_e \tag{4}$$

3. The Exact Solution of the BVP for the Canonical Equation of State (EOS) of Mobile Charges

Differentiating Eq. 3, we get the equation

$$\frac{d\varphi}{dz} = -\frac{a_e^2}{\sigma_e}\frac{d\rho_e}{dz} \tag{5}$$

where a_e^2 is defined as

$$a_e^2 \equiv \left(\rho\psi\right)_{\rho_e\rho_e} \tag{6}$$

and $\psi\left(\rho_e\right)$ is the energy per unit mass of the negatively charged liquid of mobile particles. Here and in the following we assume that the conductor is maintained at fixed temperature and skip the T parameter.

Generally speaking, the quantity a_e^2 is a nonlinear function of the density ρ_e. This fact makes the electrostatic problem an essentially nonlinear partial differential equation, the solution of which is hard to find analytically.

Following Grinfeld and Grinfeld,[5] consider the particularly simple, but instructive case when the function $a_e^2 \equiv (\rho e)_{\rho_e \rho_e}$ is a positive constant. In this case, inserting Eq. 5 in the equation of electrostatics, Eq. 2, we arrive at the following linear ordinary equation:

$$\frac{a_e^2}{4\pi\sigma_e}\frac{d^2\rho_e}{dz^2} = \sigma_e\rho_e + \sigma_i\rho_i \tag{7}$$

Looking for the solutions of Eqs. 6 and 7 in the form

$$\rho_e = A_e e^{\lambda z} - \frac{\sigma_i}{\sigma_e}\rho_i \tag{8}$$

where A_e is a nonzero constant, we arrive at the algebraic equation

$$\left(\sigma_e - \frac{a_e^2}{4\pi\sigma_e}\lambda^2\right)A_e = 0 \tag{9}$$

Equation 9 leads to the following values of λ:

$$\lambda_\pm = \pm\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}} \tag{10}$$

Combining Eqs. 8 and 9, we arrive at the following general solution of our problem

$$\rho_e(z) = -\frac{\sigma_i}{\sigma_e}\rho_i + A_+ e^{\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}z} + A_- e^{-\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}z} \tag{11}$$

where A_+ and A_- are the (arbitrary) constants to be determined from the additional conditions.

Equation 11 leads us to the following relationship for the local charge distribution:

$$\sigma_e\rho_e(z) = -\sigma_i\rho_i + A_+\sigma_e e^{\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}z} + A_-\sigma_e e^{-\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}z} \tag{12}$$

If we are looking for a solution that is symmetric with respect to the point $z = 0$, we have to demand that

$$A_+ = A_- = A \tag{13}$$

Then the general solution, Eq. 11, for the symmetric solutions takes the form

$$\rho_e(z) = -\frac{\sigma_i}{\sigma_e}\rho_i + 2A\cosh\left(\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}z\right) \tag{14}$$

Inserting Eq. 11 into the mass balance Eq. 4, we arrive at the relationship

$$M_e = -\frac{\sigma_i}{\sigma_e}\rho_i 2H + A_+ \frac{1}{\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}}\left(e^{\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}H} - e^{-\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}H} \right) - A_- \frac{1}{\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}}\left(e^{-\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}H} - e^{\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}H} \right) \tag{15}$$

We can rewrite Eq. 15 as

$$M_e = -\frac{\sigma_i}{\sigma_e}\rho_i 2H + 2\left(A_+ + A_-\right)\frac{1}{\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}}\sinh\left(\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}H\right) \tag{16}$$

For symmetric solutions, Eq. 16 implies

$$M_e = -\frac{\sigma_i}{\sigma_e}M_i + 4A\frac{1}{\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}}\sinh\left(\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}H\right) \tag{17}$$

Equation 17 implies the following relationship for the full charge $Q = Q_e + Q_i$, where $Q_e \equiv M_e\sigma_e$ and $Q_i \equiv M_i\sigma_i$:

$$Q_e + Q_i = 4A\sqrt{\frac{a_e^2}{4\pi}}\sinh\left(\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}H\right) \tag{18}$$

Using Eq. 18, we get the following formula for the constant A:

$$A = \frac{\sqrt{\pi}}{2a_e\sinh\left(\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}H\right)}\left(Q_e + Q_i\right) \tag{19}$$

Inserting Eq. 19 into Eq. 14, we get the following solution:

$$\rho_e\left(z\right) = -\frac{\sigma_i}{\sigma_e}\rho_i + \frac{\sqrt{\pi}}{a_e}\left(Q_e + Q_i\right)\frac{\cosh\left(\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}z\right)}{\sinh\left(\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}H\right)} \tag{20}$$

This is our exact solution. We see that the 3-D mass density of the mobile charges is a finite quantity everywhere inside the conductor.

4. On the Local Extinction of the Mobile Component

Per Eq. 20, the boundary values of the density at $z = \pm H$ are equal to

$$\rho_e(\pm H) = -\frac{\sigma_i}{\sigma_e}\rho_i + \frac{Q_e + Q_i}{a_e}\frac{\sqrt{\pi}}{\tanh\left(\sqrt{\frac{4\pi\sigma_e^2}{a_e^2}}H\right)} \tag{21}$$

At sufficiently large $|\sigma_e| H / a_e$ Eq. 21 can be replaced with

$$\rho_e(\pm H) = -\frac{\sigma_i}{\sigma_e}\rho_i + \sqrt{\pi}\frac{Q_e + Q_i}{a_e} \tag{22}$$

Per Eq. 22, when the full charge $Q_{tot} \equiv Q_e + Q_i$ is negative and has sufficiently high absolute value, the local mass density $\rho_e(H)$ can vanish. This phenomenon we call the local extinction of the electronic gas. The local extinction phenomenon requires a more delicate analysis and will be done elsewhere. It does not happen, though, when the conductor is nearly neutral (i.e., $|Q_i / Q_e| = 1 \pm \varepsilon$, where $\varepsilon << 1$).

5. Calculation of the Pressure

If we consider the isothermal processes at $T = T_0$, where T_0 is the base temperature, we arrive at the relationships

$$\psi_e(\rho_e) - \psi_{e0} = a_e^2 \frac{1}{2\rho_e}(\rho_e - \rho_{e0})^2 + p_{e0}\left(\frac{1}{\rho_{e0}} - \frac{1}{\rho_e}\right) \tag{23}$$

and

$$p_e(\rho_e) = a_e^2 \frac{1}{2}\left(\rho_e^2 - \rho_{e0}^2\right) + p_{e0}, \ (\rho\psi_e)_{\rho\rho} = a_e^2 = const \tag{24}$$

Using the Eq. 20, we get

$$p_e(z) = \frac{a_e^2}{2}\left\{\left[-\frac{\sigma_i}{\sigma_e}\rho_i + \frac{\sqrt{\pi}}{a_e}(Q_e + Q_i)\frac{\cosh\left(\sqrt{4\pi\sigma_e^2 a_e^{-2}}z\right)}{\sinh\left(\sqrt{4\pi\sigma_e^2 a_e^{-2}}H\right)}\right]^2 - \rho_0^2\right\} + p_0 \tag{25}$$

6. Conclusion

We suggested a thermodynamically consistent model of conductor (i.e., the model based on the minimum energy principle and for which the 3-D densities of the positive and negative charges remain finite everywhere inside the conductor. Of course this model drastically differs from the classical electrostatic model of conductor, the specific feature of which is the appearance of the boundary layers of charges with the infinite 3-D densities of the positive or negative charges.

7. References

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List of Symbols, Abbreviations, and Acronyms

1-D	1-dimensional
2-D	2-dimensional
3-D	3-dimensional
BVP	Boundary Value Problem
EOS	equations of state

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