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INFLUENCE OF INTERFACE POLARIZATION ON CHARGE-CHARGE INTERACTION IN TWO-LAYER SYSTEMS

The influence of a plane interface between two semi-infinite dielectrically dissimilar insulators on the interaction of two point charges located near it has been analyzed. It was shown that their interaction is significantly modified by the polarization charges induced at the interface. In particular, if the charges are in the same medium, then the dependence of their interaction energy W on the distance D between the charges differs from the Coulomb law. At the same time, if the charges are in different media, the interaction law remains Coulombic, but with an effective dielectric constant value. Deviations from the Coulombic interaction were calculated quantitatively and investigated analytically. The maps $W(\mathbf{R}_s, \mathbf{R}_p)$ describing the profiles of W as a function of the charges' coordinates $\mathbf{R}_s$ and $\mathbf{R}_p$ are presented. The approximations of $W(D)$ were obtained and their validity was analyzed. It was concluded that in layered structures, polarization corrections should always be taken into account when studying various properties of charged entities, e.g., electrons and holes forming Wannier–Mott excitons.

Keywords: two-layer structures, dielectric mismatch, charge-charge interaction, polarization forces, non-Coulombic dependence.

1. Introduction. Historical Overview

The discovery of the inverse-square law of the electrostatic force between two isolated point charges – let them be conditionally called the source Q_s and the probe Q_2 – is rather dramatic from the historical viewpoint. In vacuum, this law looks like (in CGS units)

$$\mathbf{F}_C = Q_s Q_p \frac{\mathbf{R}_p - \mathbf{R}_s}{|\mathbf{R}_p - \mathbf{R}_s|^3}, \quad (1)$$

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where $\mathbf{R}_i$ ($i = s, p$) denote the coordinates of the charges.

The matter is that the formal discoverer of law (1) somewhere between 1771 and 1781 was Henry Cavendish. His measurements showed that [1, p. 231] “...the electric attraction and repulsion must be inversely as the square of the distance, and that when a globe is positively electrified, the redundant fluid in it is lodged intirely on its surface”. This was not unexpected for Cavendish, since it was he who investigated and experimentally confirmed Isaac Newton’s law of universal gravitation under terrestrial conditions, which exhibits the same spatial dependence as expression (1). The whole complex of electrostatic problems was carefully studied by Cavendish (see also reference [2]). For example, he was the first to in-

introduce the notions of the “degree of electrification” (later called the dielectric constant) and the capacity [1, 3]. Unfortunately, unlike other electrical research, Cavendish did not publish law (1) that he had discovered, and therefore (this is justified!) he is not considered to be its author. On the other hand, Charles-Augustin de Coulomb, who discovered law (1) later than Cavendish, published the results of his measurements and their analysis [4, 5], although the latter was less thorough than Cavendish’s. Therefore, it is quite natural that just Coulomb is called the father of the law of electrostatic interaction, which has been named after him for more than two hundred years.

It follows from Eq. (1) that the charge-charge interaction energy in vacuum equals

$$W_C = \frac{Q_s Q_p}{|\mathbf{R}_p - \mathbf{R}_s|}. \quad (2)$$

It should be emphasized that the establishment of laws (1) and (2) was a great success, since until the twentieth century scientists could not isolate elementary charged particles [6]. They even had no idea about their existence! Instead, experimentalists observed the behavior of charged *macroscopic bodies* so that the assumption of the corpuscular nature of electricity [7–11] was a bold hypothesis, correct and fruitful at the theoretical level, but not directly justified by experiment at that time. Nevertheless, the suggestion of the inverse-square law in electrostatics was stimulated by the similarity with Isaac Newton’s gravitational law [12–14] (see also textbook [15]), which has been extremely successfully applied in celestial mechanics since its discovery [16]. An analogy between gravitational attraction, on the one hand, and electrostatic repulsion or attraction, on the other hand, led to the generalization of Eq. (2) to systems of many point charges (in electrostatics, whereas the gravitational case can be formulated analogously) [17–20] so that their total potential energy obeys the following equation (it was first written by Siméon Denis Poisson [21, 22] within the framework of Newtonian gravitation):

$$\Delta\Phi = -4\pi\rho, \quad (3)$$

where ρ is the bulk charge density, and Δ is the Laplace operator. It should be noted that the modern perception of the quantity Φ in Eq. (3) as the “potential function” belongs to George Green (1828) [23], whereas Carl Friedrich Gauss in 1839 independently

introduced a similar interpretation and coined Φ as the “potential” [24].

Once formulated, Poisson’s equation (3) can be considered as the general electrostatic equation describing not only the influence of the algebraic sum of separate charges, but also the action of an arbitrary configuration of external fields of whatever origin [19, 20]. Thus, the electric-field concept emerged implicitly reflecting the short-range character of the electric force mediation between bodies in space (most clearly manifested in condensed matter). This concept was suggested by Michael Faraday [8, 9, 11, 25, 26] (see also the analysis in Refs. [27–30]).

Faraday’s “mediated action” via condensed-medium constituents [8, 9] (atoms or molecules, as was firmly established at the beginning of the twentieth century [31]) inevitably led to the modification of both Coulomb laws (1) and (2), and Poisson’s equation (3) by the introduction of the dielectric constant ε (called by Faraday the “specific inductive capacity” [3, 32]). As a result, one has

$$W_D = \frac{Q_s Q_p}{\varepsilon |\mathbf{R}_p - \mathbf{R}_s|} \quad (4)$$

instead of Eq. (2). This means that any actual electrostatic interaction in a medium different from vacuum should be considered as a many-body problem [33, 34]. Even now, this aspect is not usually emphasized in textbooks. Thus, electrostatics appears as an approximation to the actual “propagation” of electric force in the medium. Such a picture was gradually recognized by Faraday himself and especially by William Thomson (Lord Kelvin from 1892); the latter followed Green, who established relationships between the bulk and surface electrostatic properties [23]. Thomson incorporated Faraday’s considerations into a mathematical theory of electrostatics [35]. Later, those views and relevant equations were developed into the electromagnetic field theory by James Clerk Maxwell [36, 37], who emphasized [37, p. 321], “...we may regard Faraday’s conception of a state of stress in the electro-magnetic field as a method of explaining action at a distance by means of the continuous transmission of force, even though we do not know how the state of stress is produced.”

The amazing history of the development of electrostatics has been studied in detail and can be found elsewhere [3, 30, 38–44]. But it is not over, and this work should be considered a contribution to this domain.

However, taking into account the reaction of the medium to the presence of charges – in particular, the emergence of a screening polarization charge – leads to the “non-Coulomb character” (sic!) of the Coulomb interaction between the charges. Let us explain this “paradox” using a simple example of two point charges, Q_{s1} and Q_{s2} ; the latter will play the role of a polarization charge. In vacuum, the probe charge Q_p will interact with the specified charges according to the following formula different from expression (1):

$$\mathbf{F}_C = Q_{s1}Q_p \frac{\mathbf{R}_p - \mathbf{R}_{s1}}{|\mathbf{R}_p - \mathbf{R}_{s1}|^3} + Q_{s2}Q_p \frac{\mathbf{R}_p - \mathbf{R}_{s2}}{|\mathbf{R}_p - \mathbf{R}_{s2}|^3}. \quad (5)$$

There is no transformation that can transform this combination into a monomial formula of type (1). And the result of its integration also differs from expression (2). Moreover, the question arises: where should the distance to the probe charge be measured from? An additional factor here is that if all three charges are not located along the same straight line, then the direction of the force with which the source charges act on the probe charge differs from both directions from the probe to the sources. Below, it is the impossibility of representing the probe charge energy in the form of a monomial expression (2) or (4) with a power exponent of -1 that we will call the “non-Coulombicity” of the interaction law.

Thus, it is no wonder that the “non-Coulombic” behavior of the interaction between charges, in principle, should be ubiquitous, whereas expressions (1) and (2), the latter even being divided by the dielectric constant ε , are, at best, the first (maybe leading) terms in an infinite series describing electrostatic interactions in a complicated system of charges [45, 46]. We emphasize that the dielectric-constant approximation discussed below $\varepsilon = \text{const}$ of the static screening in semiconductors and insulators was a great breakthrough in the nineteenth century, whereas now the spatial dispersion of the dielectric permittivity [47–51] must be taken into account to describe the mitigating influence of the medium on the electric field of, say, charged impurities, electron-like and hole-like quasiparticles, and dipolar molecules or excitons. Those extremely important issues are well documented in the literature, although they are not of crucial relevance here, where the classical dielectric-constant approximation ($\varepsilon = \text{const}$) is sufficient to study issues relevant to our goals. To be specific, here

we want to consider static image forces in two-layer structures [20, 52–56] and their role in deviations from the Coulomb law.

The method of image forces and image charges (fictitious, they replace actual emerging polarization charges) was invented by William Thomson [57, 58] for conductors (ideal metals) and subsequently generalized to insulators [51, 59–63]. The image-charge influence on charge-charge, charge-dipole, and dipole-dipole interactions in layered systems with well-defined interfaces was extensively studied and now constitutes a routine method (see, e.g., Refs. [63–70]).

It should be noted that electrostatics itself, being a classical macroscopic theory, cannot ensure the stability of configurations containing charges (multipoles), which was first demonstrated by the Reverend Samuel Earnshaw in 1842 [71]. This and related issues continue to be studied [72–77]. On the other hand, the observed stability of matter is a consequence of quantum-mechanical effects [78, 79].

Moreover, the bulk self-energies of charges in condensed matter (“the inner potential”) become finite [66, 80–86], since the electrostatic screening removes divergences in Eqs. (1) and (2). The same is true for image force energies [80, 83, 87–89], which diverge within the framework of the theory presented in textbooks on electrostatics [20, 52–56].

Thus, the many-body character of true electrostatic forces makes them substantially weaker than the classical Coulombic ones. It means that the basic two-body laws (1) and (2) are valid only at the microscopic level, such as in the physics of the hydrogen atom, where the average distance between the nucleus and the electron equals the Bohr radius so that the macroscopic approach is not applicable, and any screening by the neighboring atoms is absent on this scale. The difference between the theoretical results of the Niels Bohr model and the experimental energy levels is rather well explained on the basis of the Paul Dirac relativistic quantum-mechanical equation [90]. At the same time, there are also tiny quantum-field corrections that lead, in particular, to the Willis Lamb shift [91] between the levels that are degenerate in the Dirac limit. This effect is due to the influence of virtual electron-positron pairs fluctuating in the electromagnetic vacuum [90, 92, 93] and can be considered as a many-body effect of higher order than the electrostatic effects discussed above.

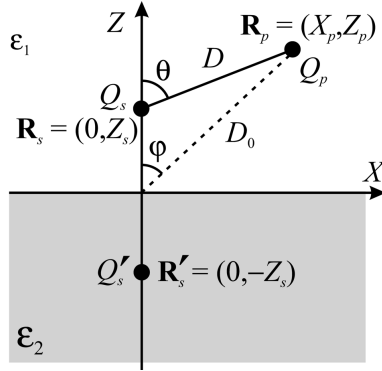


Fig. 1. Two-layer system with the interacting source charge Q_s and the probe charge Q_p . ε_1 and ε_2 are the dielectric constants of the layers (see further explanations in the text)

Interaction of a test charge with surface charges within the framework of Green's electrostatics [23], which became the interaction with mirror ghost images in Thomson's approach [35, 94], can undergo a further incarnation into the shift of the zero-point energy of surface-plasmon oscillations [95–97]. At first glance, it seems to be only a change in interpretation, but this is not the case. The description based on surface plasmons turned out to be quite fruitful. Indeed, the influence of real surface plasmons excited by *moving* test charges can lead to observable dynamic effects [53, 98–103].

From the above, it becomes clear that image forces and their influence on the spatial dependence of the Coulombic interaction between charges constitute a vast area of research. At the same time, the modest purpose of this article is twofold. First, we want to show explicitly how the polarization charges at the interfaces (for simplicity, we restrict ourselves to the planar case, bearing in mind that the spherical and cylindrical geometries are no less practically important [104–108]) distort the Coulombic interaction between charged point-like objects. And, indeed, our results demonstrate that the modifications of the bulk textbook dependences are quite significant.

Another goal is to estimate two approximation methods, in which the interaction between two point charges located in the simplest inhomogeneous system – two semi-infinite classical (dispersionless) insulators separated by a plane interface – is described by monomial formulas depending on the system parameters. In particular, it is shown that the charge-charge interaction near the inevitably polar-

ized interface demonstrates large deviations from the Coulomb-like behavior (4). This fact has been overlooked earlier and is often not properly taken into account in some textbooks and professional studies (see, e.g., [109, 110]). Within the framework of our consideration, all calculations become transparent and straightforward and can be generalized, in principle, to dipoles [61, 62, 111] and higher-order electrostatic multipoles [112]. Such an approach is in line with the spirit of the original image-charge approach in electrostatics.

The outline of the article is as follows. In Section 2, the main electrostatic formulas for two-layer dielectric structures are presented and discussed. Some general remarks concerning the calculation procedure and the presentation of its results are made in Section 3. In Sections 4, 5, and 6, the two-coordinate maps are calculated and displayed for the electrostatic energy W , the normalized energy w , and the effective dielectric permittivity ε_{eff} , respectively. The quasi-Coulombic approximation with the power exponent $N \neq -1$ is considered in more detail in Section 7. Section 8 contains conclusions.

2. Basic Electrostatic Formulas

Let us consider two homogeneous semi-infinite insulators (medium 1 and medium 2) separated by an infinitely thin interface $Z = 0$; see Fig. 1. The dielectric permittivities of the media are $\varepsilon_1 = \text{const}$ ($Z > 0$) and $\varepsilon_2 = \text{const}$ ($Z < 0$). Without any loss of generality, we may suppose that two point charges (referred to below as the source Q_s and the probe Q_p ; of course, the choice between the source and the probe is conventional) are positioned in the plane $Y = 0$. The source charge Q_s is located at a point $\mathbf{R}_s = (0, Z_s)$ in medium s . Hereafter, we use the subscript $s = 1$ or 2 for the medium where the source charge is located, and the subscript s' for the opposite medium ($s' = 2$ if $s = 1$, or $s' = 1$ if $s = 2$).

The source charge polarizes its environment. In our case, the system is inhomogeneous, i.e., it consists of two media. Therefore, in addition to the bulk polarization, which emerges in an infinitesimally small neighborhood of the charge Q_s and leads to its screening, there also emerges a polarization charge at the interface $Z = 0$. This polarization charge creates an electrostatic field in the entire space, and this field is symmetric with respect to the plane $Z = 0$. According to the classical electrostatic method applied

here, the field generated in either of the two insulators by the polarization charge distributed over their plane interface is equivalent to the field generated by an imaginary point charge (image charge) located in the other insulator [51, 59–63].

Thus, our task comes down to the problem where the source and polarization charges are fixed in an infinite medium with the dielectric permittivity ε_s . Then, in the region occupied by medium s , the polarization-induced field is equivalent to that created in an infinite medium with the dielectric permittivity ε_s by an imaginary point charge (image charge 1), which has the magnitude

$$Q'_s = K_{ss'} Q_s \quad (6)$$

and is located at the point $\mathbf{R}'_s = (0, -Z_s)$. The point $\mathbf{R}'_s$ is a specular reflection of the point $\mathbf{R}_s$, where the source charge is located, with respect to the interface as a mirror. Hence, it is positioned in the region occupied by medium s' .

The dielectric mismatch factor

$$K_{ss'} = \frac{\varepsilon_s - \varepsilon_{s'}}{\varepsilon_s + \varepsilon_{s'}} = \frac{\varepsilon_s/\varepsilon_{s'} - 1}{\varepsilon_s/\varepsilon_{s'} + 1} \quad (7)$$

in Eq. (6) depends on the ratio $\varepsilon_s/\varepsilon_{s'}$ between the dielectric constants rather than on each constant separately. The value of $K_{ss'}$ can vary from -1 to 1 , and the sign depends on the relationship $\varepsilon_s \leq \varepsilon_{s'}$. Therefore, the signs of Q_s and Q'_s can be identical or opposite. The situation with $\text{sign } Q_s = \text{sign } Q'_s$ if $\varepsilon_s > \varepsilon_{s'}$ might seem rather puzzling at first glance. However, we have to bear in mind that in the classical electrostatics one deals with two polarizable media consisting of positive and negative charges [59, 113]. The interpretation according to the adopted approach is as follows. The charge Q_s (let it be positive for definiteness) “repels” positive charges and “attracts” negative ones in both media. The “displacement” of the charges is larger in the more polarizable medium (with a larger ε). Everywhere in the bulk of both media those “shifted” charges mutually compensate one another, except at the interface. Here, the displaced uncompensated positive (!) charge in medium s is added to the displaced uncompensated negative (!) charge in medium s' . The sign of the sum depends on which value is larger, i.e., on the relationship $\varepsilon_s \leq \varepsilon_{s'}$. Actually, the interface is not an infinitely thin plane, and there is always

a surface (interface) dipole at the interface between different media, even in the absence of additional external charges [114–117]. However, accounting for the interface-dipole influence on image forces goes beyond classical electrostatics.

As a consequence, the probe point charge Q_p , if it is also located in medium s at the point $\mathbf{R}_p = (X_p, Z_p)$, interacts with both charges, Q_s and Q'_s , and the energy of this interaction equals [compare with Eq. (2)]

$$W_{ss}(\mathbf{R}_s, \mathbf{R}_p) = \frac{Q_s Q_p}{\varepsilon_s} \left(\frac{1}{|\mathbf{R}_p - \mathbf{R}_s|} + \frac{K_{ss'}}{|\mathbf{R}_p - \mathbf{R}'_s|} \right). \quad (8)$$

Thus, in essence, the mismatch factor $K_{ss'}$ determines the weight of the contribution caused by polarization charges to the total field W_{ss} and, hence, the deviation of W_{ss} from W_D (4).

At the same time, due to the symmetry of the field created by the polarization charge on both sides of the interface, the field created in medium s' is equivalent to the field created by another imaginary charge (image charge 2) with the same value Q'_s located symmetrically to image charge 1, i.e., exactly at the point $(\mathbf{R}'_s)' = \mathbf{R}_s$ in medium s where the source charge Q_s is located. Hence, the charges Q_s and Q'_s overlap at this point. As a result, there arises a total point charge

$$Q_s + K_{ss'} Q_s = \frac{2\varepsilon_s}{\varepsilon_s + \varepsilon_{s'}} Q_s$$

at the point $\mathbf{R}_s$, and we obtain one term instead of two for the interaction energy between this combined charge and the probe charge,

$$W_{ss'}(\mathbf{R}_s, \mathbf{R}_p) = \frac{2Q_s Q_p}{\varepsilon_s + \varepsilon_{s'}} \frac{1}{|\mathbf{R}_p - \mathbf{R}_s|}. \quad (9)$$

Thus, we have the exact Coulomb dependence with the effective dielectric permittivity $\frac{1}{2}(\varepsilon_s + \varepsilon_{s'})$. One should bear in mind that this is not a result of charge compensation at the point $\mathbf{R}_s$ (the charge Q'_s is imaginary), but is due to the overlap of two electric fields created by the charge Q_s in medium s and the polarization charge distributed over the interface.

Note that Eq. (8) for W_{ss} is different for $s = 1$ or 2 when both charges are located in one medium. In particular, $K_{12} = -K_{21}$. On the contrary, for the charges located in different media ($s \neq s'$), Eq. (9) does not allow one to determine which charge is the source or the probe, as required by the symmetry of the problem.

2.1. A variant of the image force method

As described above, in the classical image method, the calculation of the interaction of two point charges near a plane interface between two infinite homogeneous dielectrics is reduced to the calculation of the interaction of three charges in a homogeneous infinite medium with the dielectric constant ε_s . These are the source charge Q_s , the probe charge Q_p , and the imaginary charge Q'_s , which creates the same field at the probe location as the polarization charge at the interface does. In so doing, the polarization charge created at the interface is not taken into account. In any case, the magnitude of the image charge (6) depends on the ratio $K_{ss'}$ between the dielectric constants of both media. This is a certain inconvenience when considering more complex systems (e.g., multilayer structures) and multipoles (e.g., dipoles).

However [118], “*There are nine and sixty ways of constructing tribal lays, and every single one of them is right!*” Therefore, we will demonstrate that it is technically quite convenient to analyze the physics of the process in another model [69].

Thus, expression (4) can be formally considered as corresponding to the interaction of charges Q_s and Q_p in a medium with a dielectric constant ε . Or it can be considered as describing the interaction of charges Q_s and Q_p/ε in a medium with a dielectric constant of 1. Such variants always exist. That is, the effect on charges due to their screening can be reduced to introducing the effective dielectric constant of the medium, whereas the charges themselves are considered unchanged.

Let us apply this to expression (8) for charges located in the same medium. It can be interpreted as the interaction of unshielded charges Q_s and Q_p through two channels: both are infinite dielectrics, but one of them (the first term) has the dielectric constant ε_s (here the charge Q_p is located at the point $\mathbf{R}_p$, and the charge Q_s at the point $\mathbf{R}_s$), and the other (the second term) has the dielectric constant $\varepsilon_s/K_{ss'}$ (here the charge Q_p is also located at the point $\mathbf{R}_p$, but the charge Q_s is at the point $\mathbf{R}'_s$). In the case when the charges are in different media, their interaction can also be considered as occurring through the same two channels. But, as was already mentioned above, in the first channel the charge Q'_s is located symmetrically to Q_s with respect to the interface, and in the second channel, it coincides with

Q_s . As a result, in the second case, two identical interaction channels (the multiplier $|\mathbf{R}_p - \mathbf{R}_s|^{-1}$) arise in a homogeneous medium with the dielectric constant ε_s , but these channels have different weights, 1 and $K_{ss'}$. By adding them, we obtain formula (9), and can interpret it as the interaction of charges Q_s and Q_p (they also remain unchanged!) in a single effective channel, which is an infinite dielectric with the dielectric permittivity $\frac{1}{2}(\varepsilon_s + \varepsilon_{s'})$.

3. Some Remarks Before Calculations

Here, we have to point out the following circumstances. In order to study the deviations from the Coulomb law, we analyze two-dimensional $[\mathbf{R}_p = (X_p, Z_p)$ at $\mathbf{R}_s = \text{const}]$ maps of various quantities characterizing the interaction of two point charges in a two-layer system (see Fig. 1). These are the interaction energy W itself, its normalized variant w , and two quantities, the effective dielectric constant ε_{eff} and the effective power exponent N , which can be and are used for the pseudo-Coulombic approximation of the real W -dependence. We also intend to trace how those maps depend on the problem parameters. The W -maps are described by Eqs. (8) and (9), which depend on the individual values of the quantities ε_s , $\varepsilon_{s'}$, and the product $Q_s Q_p$, whereas the formulas for other maps can be presented in forms that include only the ratio $\varepsilon_s/\varepsilon_{s'}$ or the parameter $K_{ss'}$ [Eq. (7)].

Therefore, from the very beginning, we assumed that

$$Q_s Q_p = 1, \quad (10)$$

which is some kind of normalization. (In order to avoid troubles with measurement units, we chose arbitrary units for all quantities: charges, distances, and energies.) To trace the dependences of the maps on the dielectric parameters ε_s and $\varepsilon_{s'}$, we plotted the maps for two variants:

$$(\varepsilon_1 = 1, \varepsilon_2 = 2) \Rightarrow K_{12} = -\frac{1}{3} \quad (11)$$

and

$$(\varepsilon_1 = 1, \varepsilon_2 = 5) \Rightarrow K_{12} = -\frac{2}{3}. \quad (12)$$

The set $(\varepsilon_1, \varepsilon_2)$ is relevant to the W -maps, and the mismatch factor K_{12} is relevant to all other maps. The maps were calculated for both variants. Qualitatively, those maps are similar in pairs. Therefore,

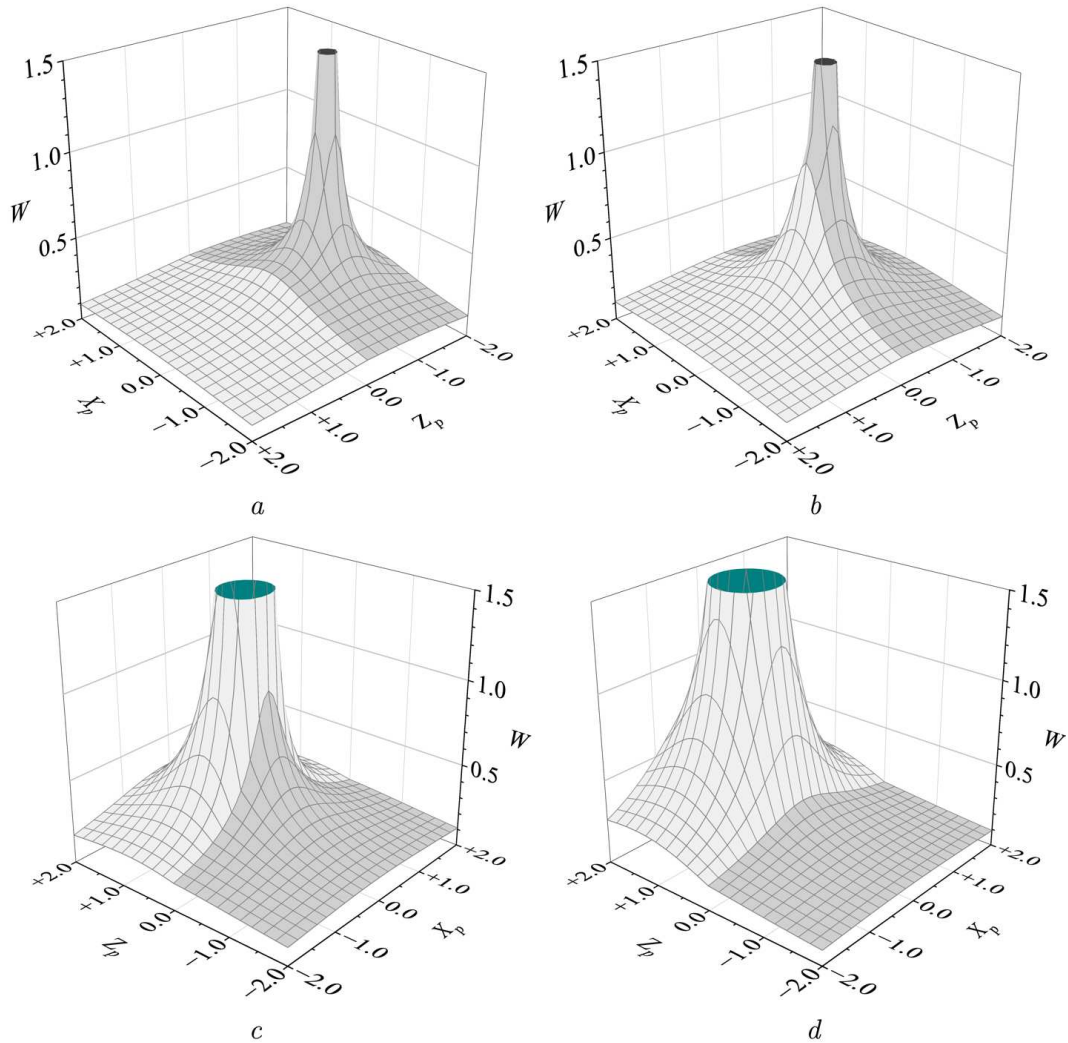


Fig. 2. W -maps, where W is the interaction energy (in arbitrary units) between Q_s and Q_p for various Q_s -locations $\mathbf{R}_s = (X_s = 0, Z_s)$: $Z_s = -1$ (a), $-\frac{1}{3}$ (b), $\frac{1}{3}$ (c), and 1 (d). $\varepsilon_1 = 1$, $\varepsilon_2 = 5$. The map region corresponding to medium 1 (2) is lighter (darker). In this figure, panels a and b are rotated with respect to panels c and d around the W -axis to make the map peculiarities clearer

for the illustration of each map evolution, we selected the variant that, in our opinion, better demonstrates the map's peculiarities.

4. W -Maps

First, let us consider the map $W(X_p, Z_p) = W_{ij}(\mathbf{R}_s, \mathbf{R}_p)$ describing the interaction of two point charges when the source charge is located at the point $\mathbf{R}_s = (X_s, Z_s)$ and trace the evolution of this map when the source charge moves perpendicularly

to the interface. It is enough to examine the particular case $X_s = 0$, when the charge Q_s is positioned on the X -axis. This map has a singularity $O(D^{-1})$ at the source-charge location $\mathbf{R}_s$, where $D = |\mathbf{R}_p - \mathbf{R}_s|$ is the probe-to-source distance. The evolution of this singularity (and the map in general) with the change of the source-charge position for parameter set (10), (12) is illustrated in Fig. 2.

Returning to Fig. 1, if the distance D between the charges is small, the contribution of polarization charges (the second term in Eq. (8)) is negligible so

that the dependence $W_{ij}(\mathbf{R}_s, \mathbf{R}_p)$ becomes almost Coulomb-like. The proximity of the source charge to the interface, where the W -surface has a kink, distorts the smoothness and symmetry of the map. The singularity's cross-section is no longer a circle, but it is very close to it. One can observe this in Fig. 2, where the cross-sections (tinted in dark gray) are made at the arbitrarily chosen level $W_0 = 1.5$. Furthermore, if $Z_s = 0$, the singularity restores its exact Coulomb-like character. Therefore, we can roughly (see Section 6) estimate the “radius” R_0 of this singularity at a certain energy level W_0 using the relationship

$$W_0 = \frac{Q_s Q_p}{\varepsilon_s R_0}. \quad (13)$$

Here ε_s is the dielectric permittivity of the s th ($s = 1, 2$) medium where the source charge is located. If the source charge is at the interface, the Coulomb law is applicable for any D , with the effective dielectric permittivity being equal to $\frac{1}{2}(\varepsilon_1 + \varepsilon_2)$. Thus, the “effective radii” of the W -singularity for the source-charge positions “deeply in medium 1”, “at the interface”, and “deeply in medium 2” are related as $\frac{1}{\varepsilon_1} : \frac{2}{\varepsilon_1 + \varepsilon_2} : \frac{1}{\varepsilon_2}$.

5. Normalized w -Maps

Based on the evolution of W -map singularity (see Section 4), one may expect that this singularity smoothly retains its true Coulombic character (4) at least in the source-charge vicinity because the polarization contribution is finite here, whereas the direct source–probe interaction diverges. This hypothesis can be confirmed or discarded by normalizing the map $W(X_p, Z_p)$ by the true Coulombic dependence (4), where ε is a relevant dielectric constant. Then, if the hypothesis is valid, the normalized map $w = W/W_C$ should be represented by an almost flat surface or, at least, a round dome in the vicinity of the singularity. As for the parameter ε in Eq. (4), we selected the averaged one $\varepsilon = \frac{1}{2}(\varepsilon_1 + \varepsilon_2)$ for two reasons. First, if the charges are in different media, then, according to Eq. (9), the result will not depend on where the source charge is located (recall that we intend to trace the map evolution as the source charge “moves” from one medium into another); therefore, the normalized map will always be a flat plane $w = 1$ in the corresponding regions, which simplifies the analysis. Second, it is easy to show that

expression (8) tends to expression (9) if $|\mathbf{R}_p| \rightarrow \infty$; we will discuss this below. Additionally, as was indicated above, this normalization excludes not only the charge values Q_s and Q_p but also the constants ε_1 and ε_2 as separate entities from further consideration. The required parameter set is reduced to a single parameter $\varepsilon_1/\varepsilon_2$ or K_{12} .

In Fig. 3, the normalized-map evolution is depicted for $K_{12} = -\frac{2}{3}$ ($\varepsilon_1/\varepsilon_2 = \frac{1}{5}$). The normalized map contains a cone rather than a wrongly expected flat surface at the source-charge location.

Nevertheless, such a behavior is quite explainable. Let us consider expression (8) in the vicinity of the source-charge location $\mathbf{R}_s$ for the charges located on the same normal to the interface. The first term in parentheses has a singularity, but the second one is a smooth dependence on the difference $D = Z_p - Z_s$. Expanding it in a series of D , we obtain

$$W_{ss}(Z_s, Z_p) = \frac{A}{|Z_p - Z_s|} + B + C_1(Z_p - Z_s) + O[(Z_p - Z_s)^2].$$

The normalization of this expression by expression (4) gives

$$w_{ss}(Z_s, Z_p) = A' + B'|Z_p - Z_s| + O[|Z_p - Z_s|(Z_p - Z_s)]. \quad (14)$$

If the charges are equidistant from the interface, then

$$W_{ss}(X_s, X_p) = \frac{A}{|X_p - X_s|} + B + C_2(X_p - X_s)^2 + O[|X_p - X_s|(X_p - X_s)^2]$$

and

$$w_{ss}(X_s, X_p) = A' + B'|X_p - X_s| + O[|X_p - X_s|(X_p - X_s)^2]. \quad (15)$$

It is the second term in expressions (14) and (15) that is responsible for the conical character of the w -map in the vicinity of $\mathbf{R}_s$.

A characteristic feature of this peculiarity is the constancy of its maximum deviation at $\mathbf{R}_p = \mathbf{R}_s$ from the plane $w = 1$; this deviation is different for $Z_s \leq 0$. Indeed, from formulas (8) and (4) with

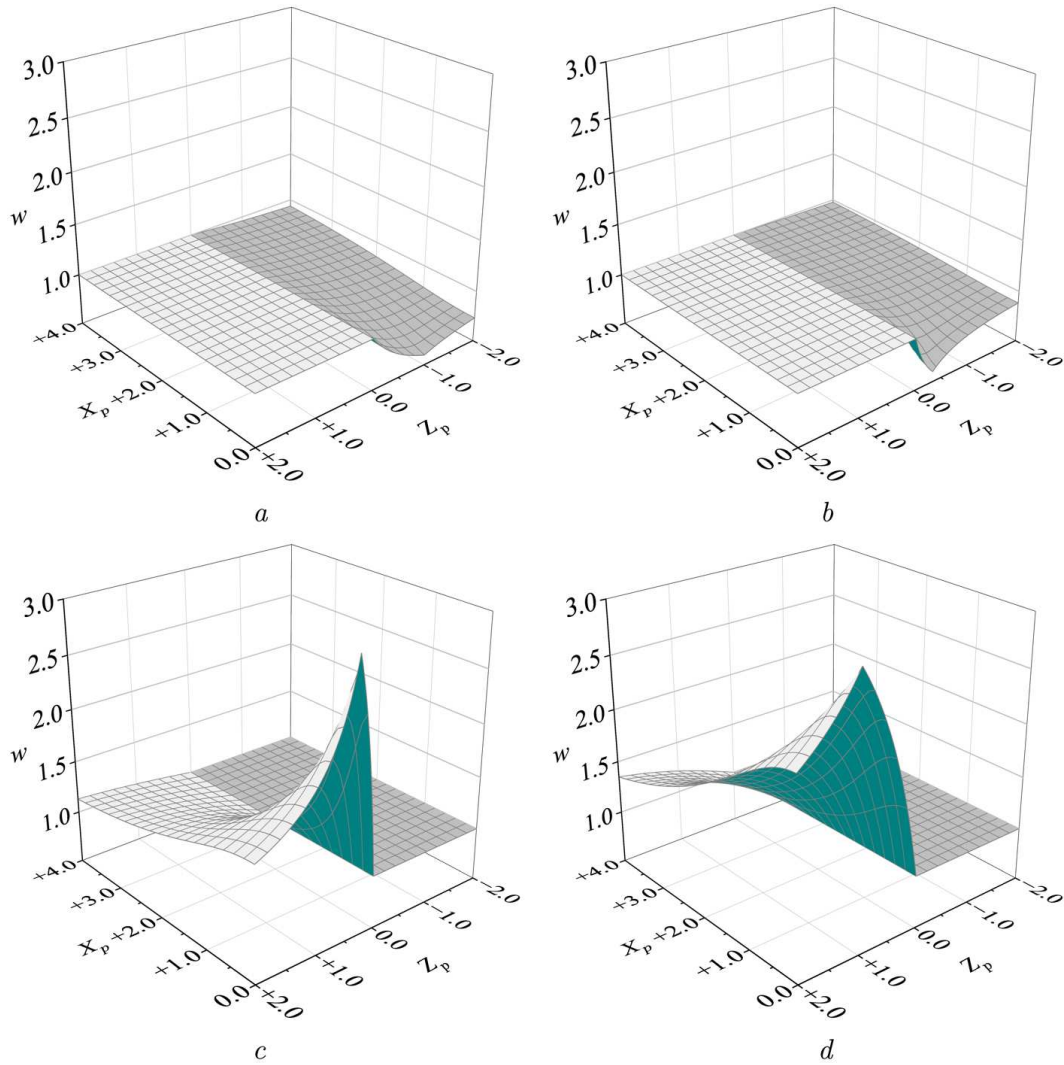


Fig. 3. Normalized w -maps for $K_{12} = -\frac{2}{3}$ ($\varepsilon_1/\varepsilon_2 = \frac{1}{5}$). $Z_s = -1$ (a), $-\frac{1}{3}$ (b), $\frac{1}{3}$ (c), and 1 (d)

$\varepsilon = \frac{1}{2}(\varepsilon_1 + \varepsilon_2)$, the following expression for the normalized quantity w can be obtained:

$$w(X_p, Z_p) = \frac{1}{K_{ss'} + 1} \left(K_{ss'} \frac{\sqrt{X_p + (Z_p - Z_s)^2}}{\sqrt{X_p + (Z_p + Z_s)^2}} + 1 \right). \quad (16)$$

As a result, its maximum deviation in medium s equals

$$\max \Delta w_s = \lim_{X_p \rightarrow 0, Z_p \rightarrow Z_s} w(X_p, Z_p) - 1 = -\frac{K_{ss'}}{K_{ss'} + 1}. \quad (17)$$

It depends only on the parameter $K_{ss'}$, whereas the dependence on Z_s disappears. In particular, if both charges are in medium $s = 1$, then for the chosen value $K_{12} = -\frac{2}{3}$, the maximum difference has a peak at $\mathbf{R}_p = \mathbf{R}_s$, which equals 2; cf. Figs 3, a and 3, b. But if both charges are in medium $s = 2$, then $K_{21} = \frac{2}{3}$, and the maximum difference from the level $w = 1$ has a dip equal to $-\frac{2}{5}$ at $\mathbf{R}_p = \mathbf{R}_s$; cf. Figs 3, c and 3, d. As follows from formula (17), the ratio between the peak height and the dip depth equals ($K_{21} = -K_{12}$)

$$\frac{\max \Delta w_{s=1}}{\max \Delta w_{s=2}} = \left| \frac{-\frac{K_{12}}{K_{12}+1}}{-\frac{K_{21}}{K_{21}+1}} \right| =$$

$$= \frac{1 - K_{12}}{1 + K_{12}} = \frac{\varepsilon_2}{\varepsilon_1}, \quad (18)$$

which equals 5 for $K_{12} = -\frac{2}{3}$.

Thus, the direction of w -surface deviation from the reference plane $w = 1$ is determined by the sign of $K_{ss'}$. This is a result of whether the signs of the source charge Q_s and the polarization charge at the interface coincide or not; see Section 2. The probe charge begins to feel the polarization charge even when located in the vicinity of Q_s . If $\varepsilon_s < \varepsilon_{s'}$, the signs of the source and polarization charges coincide, the energies of the probe interaction with them are summed, their sum exceeds the interaction energy between the probe and the source, and one obtains a peak. But if $\varepsilon_s > \varepsilon_{s'}$, the signs of the source and polarization charges are different, the energy of the interaction between the probe and the polarization charge is subtracted from the probe-source interaction energy, the result is lower than the net probe-source interaction energy, thus creating a dip.

At $Z_s = 0$, Eq. (16) gives a flat surface $w(X_p, Z_p) = 1$. This is a limit to which expression (16) tends nonuniformly as $Z_s \rightarrow -0$ and $Z_s \rightarrow +0$. It is this nonuniformity that is responsible for the presence of the cusp in the normalized maps calculated for $Z_s \neq 0$. This fact testifies that it is not valid to use the classical Coulombic dependence (4) to describe the electrostatic interaction between two point charges near the interface between dielectrically different media. The deviation from Eq. (4) remains significant even if the charges concerned are located close to each other: it has the first-order smallness rather than the second-order one in the source-to-probe distance. This is important, e.g., for the Wannier-Mott exciton or trion formation in layered systems [119–121].

6. Effective Dielectric Permittivity. ε_{eff} -Maps

Only for a confined spherically symmetric charge distribution, the potential beyond its boundaries has the exact Coulombic dependence everywhere with the power exponent $N = -1$. Such distributions really exist and are practically important [122–126]. At the same time, there is a need for simple analytical expressions for approximating the real coordinate behavior of more complicated systems, at least in a certain range of distances. This is because sometimes the

corresponding consideration allows one to obtain analytical results, which are important for further estimates and planning computations.

As concerns our system (see Fig. 1), Eq. (8) with the omitted second term is sometimes used to simplify the analysis [133, 134]; i.e., the polarization charge arising at the interface is neglected. However, even when molecular levels near the interfaces were considered taking into account the image-charge influence, the calculations were not carried out in a consistent way from the electrostatic viewpoint; see, e.g., [135, 136]. To demonstrate the importance of the interface polarization effect, let us check the validity of the simplified one-term model by plotting the (X_p, Z_p) -map of the quantity ε_{eff} satisfying the relationship

$$W_{ss'}(\mathbf{R}_s, \mathbf{R}_p) = \frac{1}{\varepsilon_{\text{eff}}} \frac{Q_s Q_p}{|\mathbf{R}_p - \mathbf{R}_s|}, \quad (19)$$

where the l.h.s. $W_{ss'}(\mathbf{R}_s, \mathbf{R}_p)$ is described by the true full expression (8). Hereafter, since the maps are symmetric with respect to the plane $X_p = 0$, we will demonstrate only the map section corresponding to $X_p \geq 0$. By doing so, we will better illustrate the map peculiarity arising at the point $\mathbf{R}_p = \mathbf{R}_s$. Now, as was described above, the parameter set consists of the single quantity K_{12} .

Figure 4 displays the ε_{eff} -maps for various positions of the source charge Q_s (recall that the specific Q_s - and Q_p -values can be arbitrary in this case) for $K_{12} = -\frac{2}{3}$ (parameter set (12)). The situation with the plateau in medium s' is clear: here, $W_{ss'}(\mathbf{R}_s, \mathbf{R}_p)$ is described by formula (9) so that the exact equality $\varepsilon_{\text{eff}} = \frac{1}{2}(\varepsilon_1 + \varepsilon_2)$ holds. It is noteworthy that if both charges are in the same medium, then $\varepsilon_{\text{eff}} = \varepsilon_s$ only at the single point $\mathbf{R}_p = \mathbf{R}_s$, where the map has a sharp conical peculiarity.

Another feature of the ε_{eff} -maps is that $\varepsilon_{\text{eff}} \rightarrow \frac{1}{2}(\varepsilon_1 + \varepsilon_2)$ as the source-to-probe distance $D = |\mathbf{R}_p - \mathbf{R}_s|$ tends to infinity. Thus, if the source is in medium 1 ($\varepsilon_1 = 1 < \varepsilon_2 = 5$) and the probe moves away from it, the value of ε_{eff} first drastically increases from $\varepsilon_{\text{eff}} = 1$ and then continues to monotonically approach the value $\varepsilon_{\text{eff}} = \frac{1}{2}(\varepsilon_1 + \varepsilon_2)$. On the other hand, if the source charge is in medium 2 ($\varepsilon_1 = 5$), then the value of ε_{eff} first drastically decreases from $\varepsilon_{\text{eff}} = 5$ and then continues to monotonically decrease to the value $\varepsilon_{\text{eff}} = \frac{1}{2}(\varepsilon_1 + \varepsilon_2)$. This trend has a simple explanation.

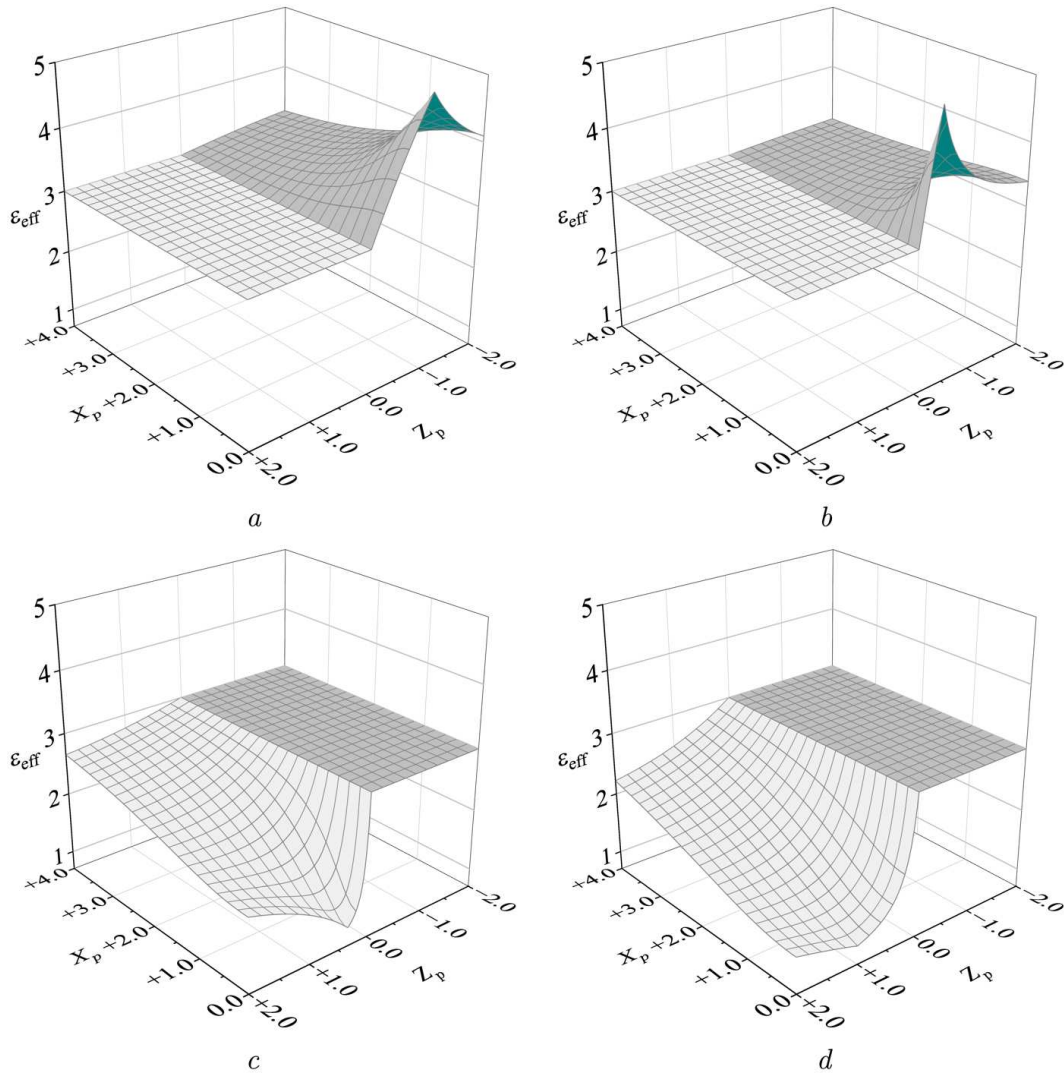


Fig. 4. ε_{eff} -maps for the same parameters as in Fig. 3

According to the consideration given in Section 2, if the source charge is in medium 1, the interaction energy is equal to the sum of interaction energies of the probe charge with both the source charge and the image charge. It is important that, according to Eqs. (6) and (7), the signs of the source charge and the image charge are different ($\varepsilon_1 < \varepsilon_2$, so $K_{12} < 0$). Very close to the source, its interaction with the probe strongly dominates (it has a Coulombic divergence) so that we can consider the second term in Eq. (8) as a small correction to the first one. However, at large distances $D \gg Z_s$, the contributions of both terms

become comparable. From the viewpoint of the probe charge located far away, the field-inducing charges get closer to each other to form a combined charge with a value of $Q_s + Q'_s$, which is smaller in magnitude than Q_s ($-1 < K_{12} < 0$). Now

$$W_{ss}(\mathbf{R}_s, \mathbf{R}_p) \approx \frac{(Q_s + Q'_s) Q_p}{\varepsilon_1} \frac{1}{|\mathbf{R}_p - \mathbf{R}_s|}, \quad (20)$$

and within the framework of the ε_{eff} -approach, one can approximately consider

$$\frac{(Q_s + Q'_s)}{\varepsilon_1} \approx \frac{Q_s}{\varepsilon_{\text{eff}}}.$$

Then

$$\varepsilon_{\text{eff}} \approx \varepsilon_1 \frac{Q_s}{Q_s + Q'_s} = \frac{\varepsilon_1}{1 + K_{12}} > \varepsilon_1. \quad (21)$$

However, if the source charge is in medium 2 ($\varepsilon_{s=2} = 5 > \varepsilon_{s'=1} = 1$), the same examination yields the relationship

$$\varepsilon_{\text{eff}} \approx \frac{\varepsilon_2}{1 + K_{21}} < \varepsilon_2 \quad (22)$$

because now $K_{21} = -K_{12} > 0$.

It is important to note that the ε_{eff} -map is the “inverse” w^{-1} -map multiplied by the factor $\frac{1}{2}(\varepsilon_1 + \varepsilon_2)$. So the existence of regions where $\varepsilon_{\text{eff}} = \text{const}$ and the conical behavior of the map at $\mathbf{R}_p \rightarrow \mathbf{R}_s$ receive a proper explanation.

As the ε_{eff} -maps show, in the analyzed geometry, the ε_{eff} -approximation is exact in the case where the charges are located in different media. Otherwise, the region in medium s where $\varepsilon_{\text{eff}} \approx \varepsilon_s$ is located rather far from the source charge, and we have $\varepsilon_{\text{eff}} \neq \varepsilon_s$ over the whole medium s . Therefore, we may conclude that in this case, the applied ε_{eff} - and ($\varepsilon = \varepsilon_s = \text{const}$)-approaches sometimes give only rough approximations of the sought dependence $W(\mathbf{R}_s, \mathbf{R}_p)$.

7. Quasi-Coulombic Approximation

7.1. N -maps

Based on our previous analysis [63,65], let us examine the following quasi-Coulombic approximation of the electrostatic dependences obtained above:

$$W(D) \approx CD^N. \quad (23)$$

Here, the parameters C and N depend on the positions $\mathbf{R}_s$ and $\mathbf{R}_p$ of both charges. Let us switch to the polar coordinate system with the origin at the point $\mathbf{R}_s$ (see Fig. 1). Then C and N are some functions of the source-to-probe distance D and the angle θ , $C(D, \theta)$ and $N(D, \theta)$. For a fixed θ_* -value, we may assume that within some D -interval around the distance D_* , C and N change insignificantly, so they can be considered as constants, C_* and N_* , respectively. If the “actual” dependence $W(D, \theta_*)$ is known, the C_* - and N_* -values can be calculated using the equations

$$N_* = \left[\frac{D}{W} \frac{dW}{dD} \right]_{D=D_*}, \quad (24)$$

$$C_* = \left[\frac{W}{D^{N_*}} \right]_{D=D_*}. \quad (25)$$

Hence, there arises the question whether there is a certain N -value in Eq. (23) that would make it at least approximately applicable to our problem. For this purpose, we should construct the map $N(X_p, Z_p)$. Owing to the simplicity of the problem, the required map can be obtained in analytical form.

In particular, if the charges are in different media, formula (24) is applied to expression (9), and the N -map in medium s' is the plane $N(X_p, Z_p) = -1$. If the point (X_p, Z_p) is located in medium s at the distance D from the source charge, and the segment connecting the charges is oriented at the angle θ with respect to the Z -axis direction (see Fig. 1), calculations using formulas (24) and (8) yield the expression

$$N(D, \theta) = -\frac{G^3 + K_{ss'} D^2 (D + 2Z_s \cos \theta)}{G^2 (G + K_{ss'} D)}, \quad (26)$$

where

$$G = \sqrt{D^2 + 4DZ_s \cos \theta + 4Z_s^2}. \quad (27)$$

Here the parameter set is also reduced to a single ratio $\varepsilon_s/\varepsilon_{s'}$ or the parameter $K_{ss'}$. The transition from $N(D, \theta)$ to $N(X_p, Z_p)$ is trivial.

The resulting N -maps calculated for $K_{12} = -\frac{1}{3}$ ($\varepsilon_1/\varepsilon_2 = \frac{1}{2}$) and various source charge positions are shown in Fig. 5. We selected this variant for illustration because in the other case, N reaches a value of -5 at the interface, and the conical map peculiarity is badly discernible at the relevant scale. So, near the interface, we can obtain an unexpectedly large N -value, whose maximum, according to formula (26), equals

$$N(Z_s, \pi) = \frac{K_{ss'} - 1}{K_{ss'} + 1} = -\frac{\varepsilon_{s'}}{\varepsilon_s}. \quad (28)$$

The validity of formula (26) in this case can be demonstrated as follows. Based on Eq. (24), let us examine the ratio (recall that $D = Z_s - Z_p$)

$$\begin{aligned} \frac{N(D \rightarrow Z_s - 0, \pi)}{N(D \rightarrow Z_s + 0, \pi)} &= \\ &= \frac{\lim_{D \rightarrow Z_s - 0} \frac{D}{W_{ss}}}{\lim_{D \rightarrow Z_s + 0} \frac{D}{W_{ss'}}} \times \frac{\lim_{Z_p \rightarrow +0} \frac{dW_{ss}}{dZ_p}}{\lim_{Z_p \rightarrow -0} \frac{dW_{ss'}}{dZ_p}} \end{aligned} \quad (29)$$

between the N -values at the interface on both its sides. Since the dependence $W(Z_p)$ is continuous

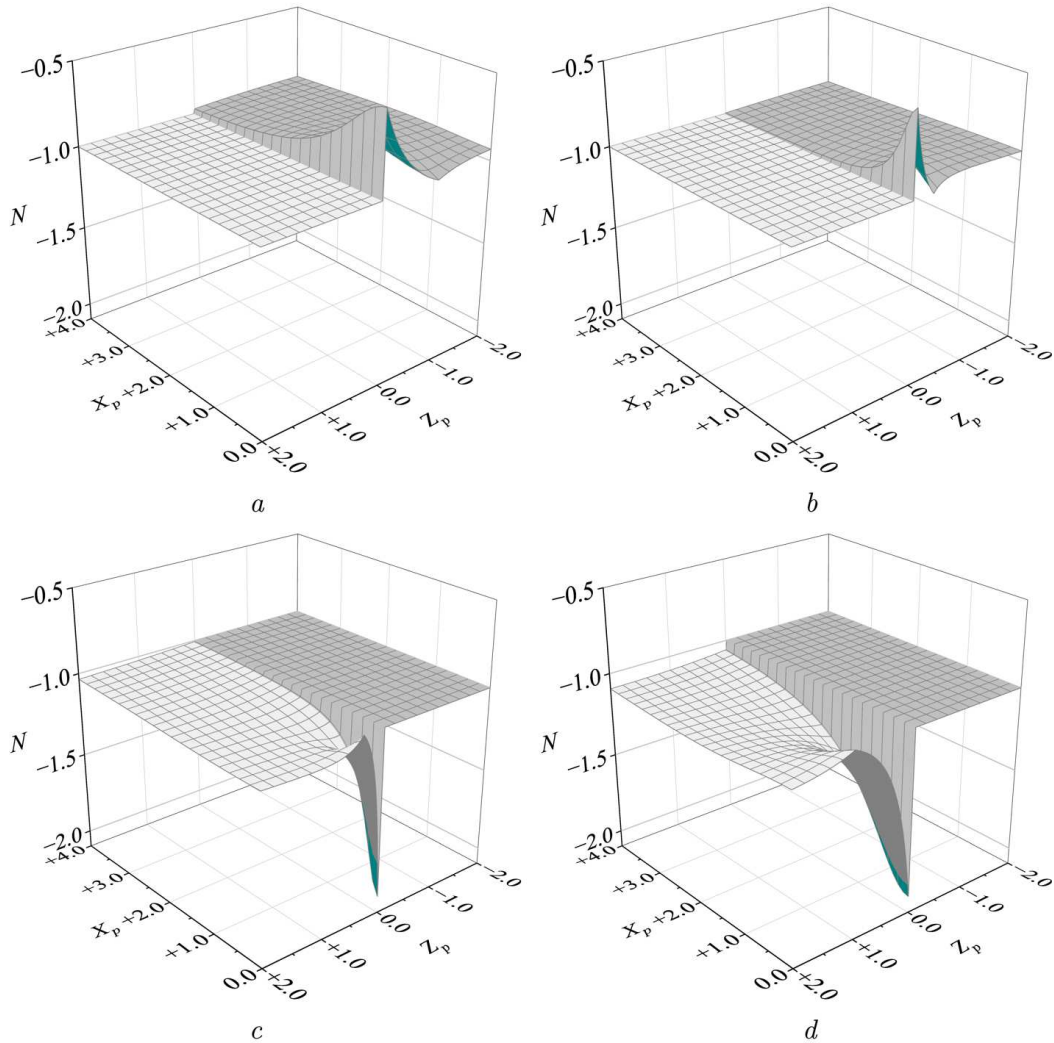


Fig. 5. N -maps for the same parameters as in Fig. 2 (see explanations in the text)

across the interface, $W_{ss}(Z_p = 0) = W_{ss'}(Z_p = 0)$, the first fraction on the right-hand side of this relationship equals 1. At the same time, the derivatives $\frac{dW_{ss}}{dZ_p}$ and $\frac{dW_{ss'}}{dZ_p}$ are proportional to the electric field values. Thus, we obtain the ratio between the electric field magnitudes across the interface, which has to be the reciprocal of the ratio between the dielectric constants of the media. Taking into account that, according to Eq. (9), the denominator $N(D \rightarrow Z_s + 0, \pi)$ on the left-hand side of Eq. (29) equals -1 , we arrive at formula (28).

The unexpected result is that the ratio $\varepsilon_{s'}/\varepsilon_s$ can, in principle, acquire any positive value. Correspondingly, the effective power exponent N can

reach any negative value $-(\varepsilon_{s'}/\varepsilon_s)$. For instance, if medium s' is a ferroelectric or a “classical” metal with $\varepsilon_{s'} \rightarrow \infty$, then N tends to infinity. The effect is similar to that found in three-layer structures [65]. Of course, this result describing the strong influence of the interface polarization (“image charges”) was obtained within the framework of classical electrostatics. However, the result will most probably survive if one takes into account the spatial dispersion of the dielectric permittivity (see, e.g., Refs. [51, 69] and references therein).

Let us examine the N -maps as a whole. One can see that in addition to medium s' , the Coulombic value $N = -1$ of the power exponent in approximation (23)

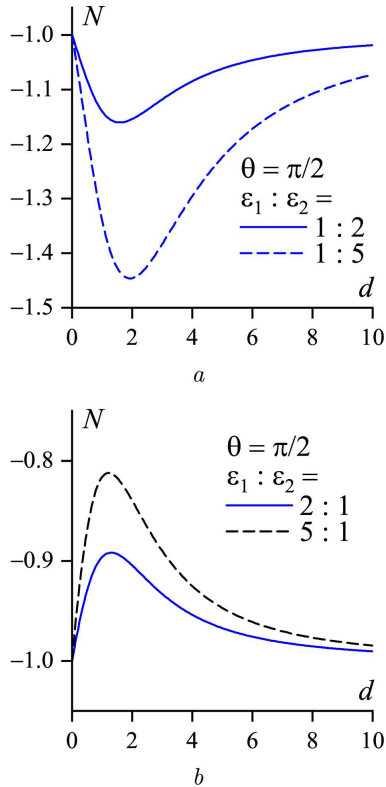


Fig. 6. Dependences of the power exponent N in Eq. (23) on the normalized distance $d = D/Z_s$ between the charges located in medium 1 equidistantly from the interface ($\theta = \pi/2$) and various ratios $\varepsilon_1 : \varepsilon_2$

for medium s is valid only at a single point $\mathbf{R}_s$ where the source charge is located. The value $N = -1$ is also reached asymptotically at infinity, $D \rightarrow \infty$, because here the Coulomb-like dependence is approached; see also Section 6. So the dependence $N(D, \theta)$ is non-monotonic in D , and the region of medium s where N substantially deviates from -1 is rather large in all directions. Hence, whether the application of the classical value $N = -1$ is sufficient as an approximation depends on the required accuracy. In any case, it should be done with caution.

The N -maps demonstrate that if the charges are located in the medium with a lower dielectric permittivity, $\varepsilon_s < \varepsilon_{s'}$, the interface polarization charge enhances the dependence of their interaction on the distance D between them in comparison with the Coulomb law, i.e., the effective $N < -1$. Otherwise, i.e., if $\varepsilon_s > \varepsilon_{s'}$, this dependence becomes weaker, $-1 < N < 0$.

7.2. Evolution of the Maps

A specific feature of the model analyzed in this work is that it has no natural length scale. Namely, the only possible length parameter is the distance $|Z_s|$ of the source charge from the interface. Therefore, if in the maps $w(X_p, Z_p)$, $\varepsilon_{\text{eff}}(X_p, Z_p)$, and $N(X_p, Z_p)$, we substitute $X_p = D_0 \sin \varphi$ and $Z_p = D_0 \cos \varphi$ (here, D_0 is the distance from the probe charge to the coordinate origin $(0,0)$; see Fig. 1) and introduce the normalization $D_0 = d_0 |Z_s|$, the obtained formulas will contain only the quantities d_0 , φ , and $K_{ss'}$ as variables; in particular, the quantity $|Z_s|$ disappears. Then, e.g., for the N -maps, we obtain

$$N(d_0, \varphi) = \frac{K_{ss'} (1 - d_0^2) k_- - k_+^3}{k_+^2 (K_{ss'} k_- + k_+)}, \quad (30)$$

where

$$k_{\pm} = \sqrt{1 + d_0^2 \pm 2d_0 \cos \varphi}.$$

In other words, for a fixed $K_{ss'}$, the resulting formulas will describe static universal maps in the normalized radial (d_0, φ) -coordinates (or the Cartesian $(x_p = X_p/|Z_s|, z_p = Z_p/|Z_s|)$ -coordinates). If the coordinate Z_s changes, the indicated maps radially deform (they shrink to the coordinate origin if $|Z_s|$ decreases, or stretch from it if $|Z_s|$ increases). As a result, all peaks and dips in medium s originating from the maps in the (X_p, Z_p) -coordinates will retain their magnitudes as they move to or from the coordinate origin. In general, as $Z_s \rightarrow 0$, we have a nonuniform convergence of the w -maps to the plane $w = 1$, the ε_{eff} -maps to the plane $\varepsilon_{\text{eff}} = 1$, and the N -maps to the plane $N = -1$. At the same time, the indicated maps in medium s' are also radially deformed. However, since they are flat in this medium, the transformation is “hidden”.

7.3. N -approximation

Now it is clear that one cannot select a certain fixed value of the parameter N in formula (23) for the latter to adequately describe the interaction between two point charges in the examined two-layer system when those charges are located in the same medium. Then, a new question arises: how well can the parameters determined by formulas (24) and (25) approximate this interaction within a finite interval of the distances between the charges?

To answer this question, let us analyze the behavior of formulas (26) and (27) when the probe charge

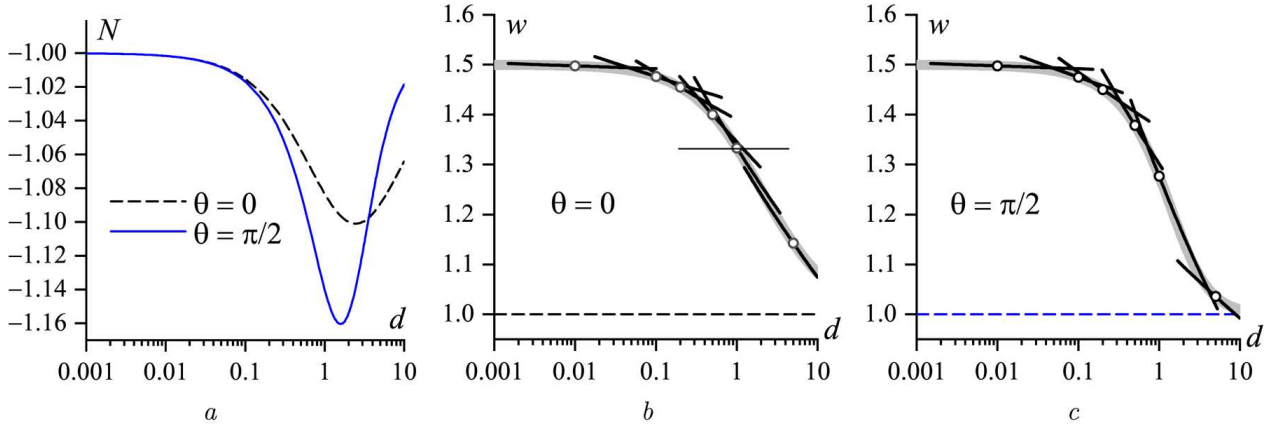


Fig. 7. *a* – comparison of the dependences $N(d)$ for charges located in medium 1 equidistant from the interface ($\theta = \frac{\pi}{2}$) and on the same normal to the interface ($\theta = 0$). *b* – dependence $w(d)$ (thick gray curve) and its approximations by quasi-Coulombic dependences (23) (solid curves) at various points on the logarithmic d scale. $\theta = 0$. The asymptotic value $w(d \rightarrow \infty)$ is shown by the dashed line. The thin horizontal line demonstrates the “genuine” Coulombic dependence ($N = -1$) calculated at $d = 1$. *c* – the same as in panel *b*, but for $\theta = \frac{\pi}{2}$. For all panels, $\varepsilon_1 : \varepsilon_2 = 1 : 2$

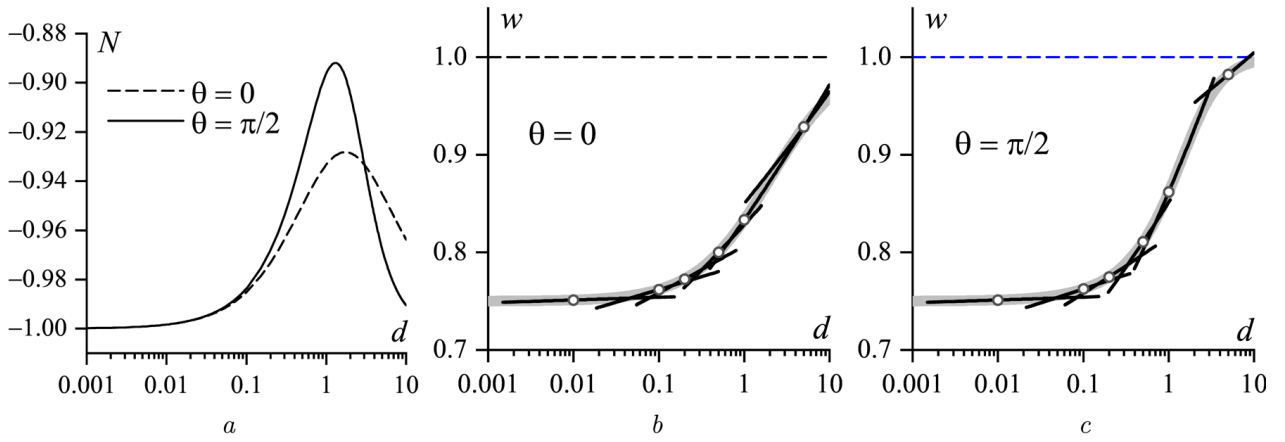


Fig. 8. The same as in Fig. 7, but for $\varepsilon_1 : \varepsilon_2 = 2 : 1$

Q_p approaches the source charge Q_s along a straight line oriented at an angle θ with respect to the normal to the interface (see Fig. 1). For simplicity, in what follows, we assume both charges to be located in medium 1 ($Z > 0, s = 1$) so that $Z < 0$ and $s' = 2$ for medium 2. Again, by normalizing the distances by $Z_s > 0$, i.e., $D/Z_s \equiv d$, the indicated formulas become universal for all $Z_s > 0$:

$$N(d, \theta) = -\frac{k^3 + K_{ss'} d^2 (d + 2 \cos \theta)}{k^2 (k + K_{ss'} d)}, \quad (31)$$

where

$$k = \sqrt{d^2 + 4d \cos \theta + 4}. \quad (32)$$

Of course, the dependence on the dimensionless factor $K_{ss'}$ is retained. Let us demonstrate the influence of $K_{ss'}$ on dependence (31). We should analyze two cases: $\varepsilon_1 < \varepsilon_2$ and $\varepsilon_1 > \varepsilon_2$. Additionally, we will restrict our analysis to the cases $\theta = 0$ (the charges are on the same normal to the interface, and the probe charge “moves” into the medium-1 depth) and $\frac{\pi}{2}$ (the charges are arranged equidistant from the interface).

In Fig. 6, the dependences $N(d, \frac{\pi}{2})$ calculated for $K_{12} = -\frac{1}{3}$ ($\varepsilon_1/\varepsilon_2 = \frac{1}{2}$) and $K_{12} = -\frac{2}{3}$ ($\varepsilon_1/\varepsilon_2 = \frac{1}{5}$) (panel *a*) and $K_{12} = \frac{1}{3}$ ($\varepsilon_1/\varepsilon_2 = \frac{2}{1}$) and $K_{12} = \frac{2}{3}$ ($\varepsilon_1/\varepsilon_2 = \frac{5}{1}$) (panel *b*) are compared. Evidently, the deviations of N from the Coulombic value $N = -1$ are larger if the media are more dielectrically differ-

ent. At the same time, the sign of deviations corresponds to the relationship $\varepsilon_1 \geq \varepsilon_2$ between the dielectric permittivities. One can see that the deviations from $N = -1$ are maximum in the practically most interesting interval $0.5 \lesssim d \lesssim 5$. Notice that the dependences shown by solid curves are the properly normalized cross-sections of the N -maps depicted in Fig. 5 by the planes drawn through the map's conical peculiarity and parallel to the (X_P, N) -plane. The results for the dependences $N(d, 0)$ are analogous, so they are not shown here.

Now we are ready to answer the question posed at the beginning of this section. From the procedure of finding the approximating dependences (23), it is clear that they are tangents to the dependences $W(D, \theta)$ at the considered reference points. So most of them have a single common point with such a dependence. The same is valid for the normalized $w(d)$ -dependences and their normalized quasi-Coulombic approximations. It is instructive to illustrate the approximations calculated for a few points located at various distances from the source point charge along the two straight lines indicated above ($\theta = 0$ and $\frac{\pi}{2}$).

In Fig. 7, we demonstrate the quality of the w -approximation (23) for $K_{12} = -\frac{1}{3}$ ($\varepsilon_1/\varepsilon_2 = \frac{1}{2}$) for $\theta = 0$ (panel *a*; the probe “goes away” from the source into the bulk of medium 1) and $\frac{\pi}{2}$ (panel *b*; the probe and the source are equidistant from the interface). Again, as in Fig. 5, the curves are the cross-sections of the corresponding maps considered above. The $(\theta = 0)$ -curves are the map cross-sections by a plane drawn through the map's conical peculiarity and parallel to the (Z_P, N) - or (Z_P, w) -plane, whereas the $(\theta = \frac{\pi}{2})$ -curves are the map cross-sections by a plane drawn through the map's conical peculiarity and parallel to the (X_P, N) - or (X_P, w) -plane.

The plotted conical peculiarities became less pronounced because they were plotted on a logarithmic d -scale (the undistorted conical profiles of the features can be seen in Fig. 6). The log scale along the d -axis was selected to include the examined points from a rather wide range of distances, $d = 0.01, 0.1, 0.2, 0.5, 1$, and 5 , which are the most interesting for practical calculations. Furthermore, the normalized approximating dependences (23) turned out to be almost linear (this is a result of the smallness of the dielectric mismatch factor R_{12}^{ε}) and clearly discernible in the chosen format. The genuine Coulombic approximation at each point would look like a

horizontal line (here, we deal with the normalized w -dependence rather than the W -one). As an example, in Fig. 7, *b*, we plotted one such approximation (at $d = 1$) by a thin solid line. Evidently, for $0 < \theta < \frac{\pi}{2}$, the corresponding curves will lie somewhere between the plotted ones.

For completeness, in Fig. 8, the same analysis was carried out for the case $K_{12} = \frac{1}{3}$ ($\varepsilon_1/\varepsilon_2 = \frac{2}{1}$), and the results obtained are very similar. Taking into account the interval of distances over which the power-like quasi-Coulombic approximation is rather satisfactory in both cases, we may conclude that this approximation can be useful in calculations.

8. Conclusions

The analysis carried out in this article within the framework of classical electrostatics shows that the interaction between two point charges located near an interface between two dielectrically different media is substantially distorted by a polarization charge induced at the interface owing to the dielectric mismatch between the media. The magnitude of the effect was estimated, and a simple approximation of the electrostatic interaction energy was proposed.

The interaction between the charges located in different media, including the case where either or both charges are at the interface, is truly Coulombic, with a modified effective dielectric permittivity.

The case where the charges are in the same medium is more interesting. Here, as the main result of calculations, we consider the conical character of the w -, ε_{eff} -, and N -maps at the point $\mathbf{R}_p = \mathbf{R}_s$, with $\varepsilon_{\text{eff}} = \varepsilon_s$ and $N = -1$ only at this point. Therefore, attempts to use the ε_{eff} - [Eq. (19)] or N_{eff} -approximation [Eq. (23)] are useful only within limited intervals of source-to-probe distances D , and the length of those intervals diminishes as the charges approach each other. It is worth noting that the deviations of N from -1 are nonmonotonic in D and strongly depend on the relationship $\varepsilon_s \lesseqgtr \varepsilon'_s$.

We emphasize that unexpected non-trivial dependences found by a thorough analysis in the basic case of a two-layer system with a dielectric mismatch clearly demonstrate that one should be very cautious when trying to apply *a priori* qualitative considerations even to simple problems. In the same research area dealing with the interface polarization and the method of image charges, a similar conclusion has

been recently drawn while resolving the paradox concerning the surface dipole moment [137].

The results obtained are of general interest and may be applied, in particular, to surface triboelectricity [125, 138] and to studies of Wannier–Mott excitons in layered systems, where the dielectric mismatch should be taken into account when calculating the binding energies [119, 127].

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ВПЛИВ ПОЛЯРИЗАЦІЇ МЕЖІ ПОДІЛУ НА ВЗАЄМОДІЮ ЗАРЯДІВ У ДВОШАРОВИХ СИСТЕМАХ

Проаналізовано вплив плоскої межі поділу між двома напівнескінченними діелектрично різними ізоляторами на взаємодію між двома точковими зарядами, розташованими поблизу неї. Показано, що їхня взаємодія суттєво змінюється поляризаційними зарядами, індукованими на межі поділу. Зокрема, якщо заряди розташовані в одному й тому ж середовищі, то залежність енергії їхньої взаємодії W від відстані D між зарядами відрізняється від кулонівської. Водночас якщо заряди розташовані в різних середовищах, закон взаємодії залишається кулонівським, але з ефективним значенням діелектричної сталості. Відхилення від кулонівської взаємодії були розраховані кількісно й досліджені аналітично. Представлено карти $W(\mathbf{R}_s, \mathbf{R}_p)$, що описують профілі W в залежності від координат зарядів $\mathbf{R}_s$ і $\mathbf{R}_p$. Отримано апроксимації $W(D)$ і проаналізовано їхню обґрунтованість. Зроблено висновок, що в шаруватих структурах поправки на поляризацію завжди слід враховувати під час вивчення різних властивостей заряджених об'єктів, наприклад, електронів і дірок, що утворюють екситони Ваньє–Мотта.

Ключові слова: двошарові структури, діелектрична невідповідність, взаємодія зарядів, поляризаційні сили, некулонівська залежність.