IMAGE (POLARIZATION) FORCES AND INTERACTION BETWEEN ELECTRIC CHARGES OR DIPOLES IN THREE-LAYER STRUCTURES

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Main recent results were published in the following articles:

[1] A. M. Gabovich, M. S. Li, H. Szymczak, A. I. Voitenko, Surf. Sci. **606** (2012) 510.
[2] A. M. Gabovich, A. I. Voitenko, Low Temp. Phys. **42** (2016) 661.
[3] A. M. Gabovich, A. I. Voitenko, Eur. J. Phys. **39** (2018) 045203.
[4] A. M. Gabovich, A. I. Voitenko, J. Molec. Liquids **267** (2018) 166.
[5] A. M. Gabovich, A. I. Voitenko, Condens. Matter **4** (2019) 44.
[6] A. M. Gabovich, M. S. Li, H. Szymczak, A. I. Voitenko, J. Electrostat. **102** (2019) 103377.
[7] A. M. Gabovich, M. S. Li, H. Szymczak, A. I. Voitenko, J. Chem. Phys. **152** (2020) 094705.
[8] A. M. Gabovich, A. I. Voitenko, J. Phys. :Condens. Matter **33** (2021) 205002.
[9] A. M. Gabovich, M. S. Li, H. Szymczak, A. I. Voitenko, Phys. Rev. B **105** (2022) 115415.

THE BIRTH OF IMAGE FORCES

William Thomson (Later Lord Kelvin), The Cambridge and Dublin Mathematical Journal, Volume III (Macmillan, Barclay, and Macmillan, Cambridge, 1848), pages 141-148, with reference to his lectures and partially unpublished works of Joseph Liouville.

* The investigations given in this paper form the subject of the first part of a series of lectures on the Mathematical Theory of Electricity, given in the University of Glasgow during the present session. They are adaptations of certain methods of proof which first occurred to me as applications of *the principle of electrical images*, made with a view to investigating the solutions of various problems regarding spherical conductors, without the explicit use of the differential or integral calculus. The spirit, if not the notation, of the *differential* calculus must enter into any investigations with reference to Green's theory of the potential, and therefore a more extended view of the subject is reserved for a second part of the course of lectures. A complete exposition of the *principle of electrical images* (of which a short account was read at the late meeting of the British Association at Oxford) has not yet been published; but an outline of it was communicated by me to M. Liouville, in three letters of which extracts are published in the *Journal de Mathématiques*, (1845 and 1847, Vols. x. and xii.) A full and elegant exposition of the method indicated, together with some highly interesting applications to problems in geometry not contemplated by me, are given by M. Liouville himself, in an article written with reference to those letters, and published along with the last of them. I cannot neglect the present opportunity of expressing my thanks for the honour which has thus been conferred upon me by so distinguished a mathematician, as well as for the kind manner in which he received those communications, imperfect as they were, and for the favourable mention made of them in his own valuable memoir.

12. ***Theorem.**** **The attraction of a uniform spherical surface on an external point is the same as if the whole mass were collected at the centre.**

The method of images concerns itself with the problem of one or more point charges in the presence of boundary surfaces, for example, conductors either grounded or held at fixed potentials. Under favorable conditions it is possible to infer from the geometry of the situation that a small number of suitably placed charges of appropriate magnitudes, external to the region of interest, can simulate the required boundary conditions. These charges are called *image charges*, and the replacement of the actual problem with boundaries by an enlarged region with image charges but not boundaries is called the *method of images*. The image charges must be external to the volume of interest, since their potentials must be solutions of the Laplace equation inside the volume; the "particular integral" (i.e., solution of the Poisson equation) is provided by the sum of the potentials of the charges inside the volume.

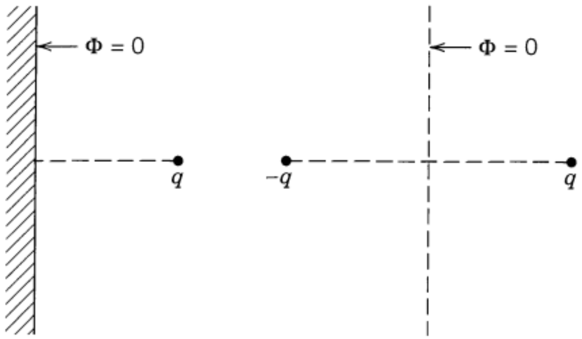
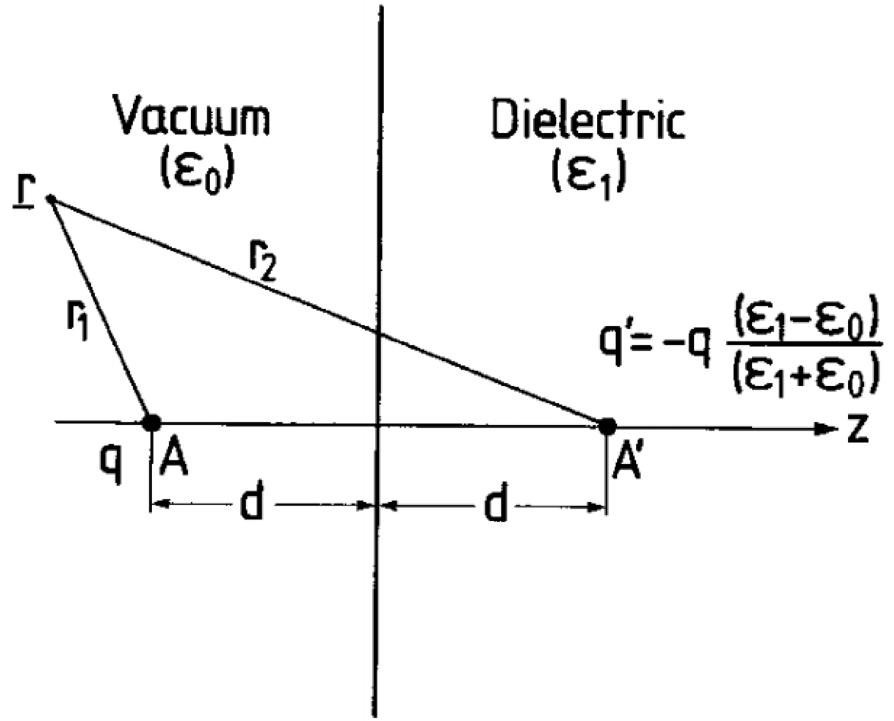


Figure 2.1 Solution by method of images. The original potential problem is on the left, the equivalent-image problem on the right.

Jackson's classical book

IMAGE (INTERFACE POLARIZATION) FORCES: PARTICULAR CASES



Method of images for a point charge outside a planar, dielectric surface

Dielectrics

P. J. JENNINGS et al.

ADVANCES IN PHYSICS, 1988, VOL. 37, NO. 3, 341–358

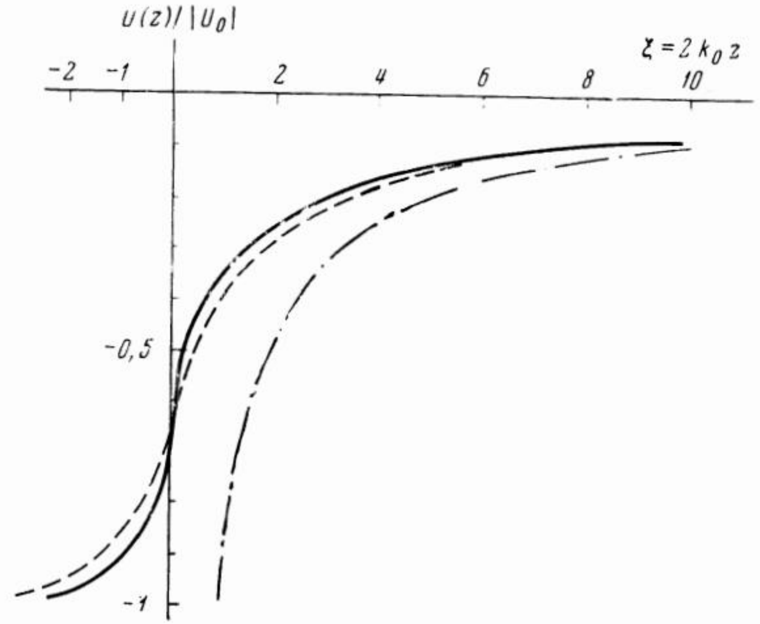


FIG. 1. The polarization contribution (18) (in the units $|U_0| = k_0e^2/2$) outside and inside of the metal. The dashed line indicates the approximation (19), and the dot-dash line is a graph of the function $-e^2/4z\,|U_0|$.

Metals. Account of screening (spatial dispersion of the dielectric permittivity) $\varepsilon(\mathbf{k},\omega)$

Specular scattering of metal electrons at its boundary

A. V. SIDYAKIN

Zh. Eksp. Teor. Fiz. 58, 573–581 (February, 1970)

IMAGE FORCE ENERGY AS CHARGE SELF-ENERGY BEING EQUAL TO TOTAL SELF-ENERGY MINUS THE BULK ELECTRON SELF-ENERGY. ANALYTICAL RESULTS IN THE QUASI-CLASSICAL THOMAS-FERMI MODEL

BULK CONTRIBUTION

$$W_{pcm}^{s-e} = W_{pc}^{s-e} - W_{scr}^{s-e}$$

$$W_{pc}^{s-e} = -\frac{q^2}{2\varepsilon}\int_0^{\infty}\frac{kdk}{k}$$

$$W_{scr}^{s-e} = -\frac{q^2}{2\varepsilon}\int_0^{\infty}\frac{kdk}{(k^2+\kappa^2)^{1/2}}$$

$$W_{pcm}^{s-e} = -\frac{q^2}{2\varepsilon}\left(\int_0^{\infty}\frac{kdk}{k} - -\int_0^{\infty}\frac{kdk}{(k^2+\kappa^2)^{1/2}}\right) = -\frac{q^2\kappa}{2\varepsilon}$$

TOTAL SELF-ENERGY (Sidyakin)

$$U(z) = \begin{cases} -\frac{e^2}{4z}\left[1+\frac{4}{\xi^2}+\pi E_2(\xi)+\pi N_2(\xi)\right], & z>0, \\ \frac{k_0 e^2}{2}\left[-1+\frac{(\xi-2)^2}{\xi^3}e^{\xi}+\frac{2}{\xi}K_2(-\xi)\right], & z<0. \end{cases}$$

where $\xi = 2k_0 z$, and $E_2(\xi)$, $N_2(\xi)$, and $K_2(\xi)$ denote the Weber, Neumann, and Macdonald functions, respectively (see, for example,[9]). For $\xi \gg 1$, i.e., $z \gg r_0$ the following expansion is valid

$$U(z) = -\frac{e^2}{4z}\left[1-\frac{2}{\xi}+\frac{4}{\xi^2}-\frac{6}{\xi^3}+\ldots\right],$$

and as $z \to 0$

$$U(z) = -\frac{k_0 e^2}{3}\left[1+\frac{3}{8}\xi\left(\ln\frac{C\xi}{2}-\frac{3}{4}\right)+\ldots\right],$$

where C is Euler's constant ($C = 0.577\ \ldots$). Outside the metal $U(z)$ varies from 0 as $z \to \infty$ to a value $(2/3)U_0$ on its surface, and inside the metal $U(z)$ rapidly reaches the limiting value $U_0 = -k_0 e^2/2$, which is the polarization contribution to the energy of a point charge in the depths of the metal using the approximation (15) for $\epsilon(k)$.

IMAGE FORCES: MORE SOPHISTICTED APPROACHES

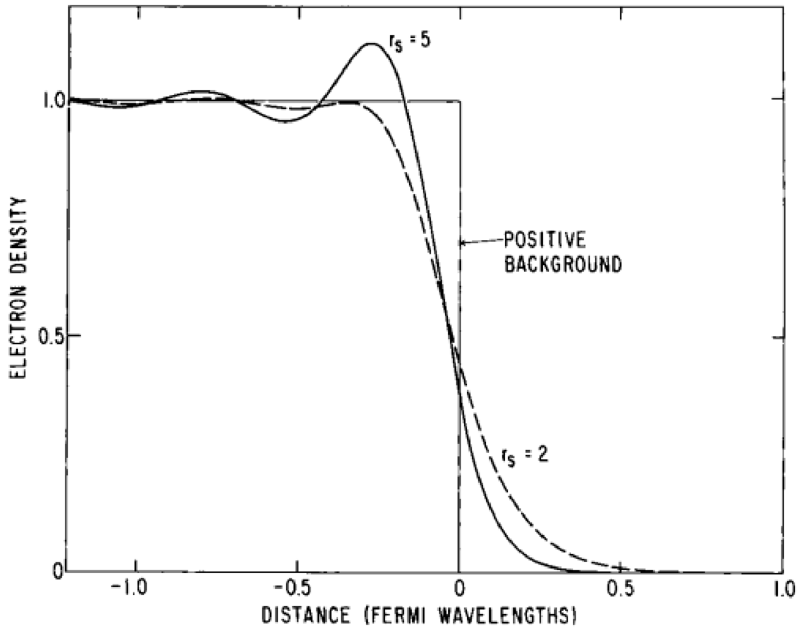


FIG. 2. Electron density at a metal surface versus distance x normal to the surface, as computed by N. D. Lang [*Solid State Commun.* **7**, 1047 (1969)] at two r_s values using the planar uniform-background model. One Fermi wavelength is equal to $2\pi/k_F$: at $r_s = 2$ this is 6.55 a.u. (3.46 Å), at $r_s = 5$ it is 16.37 a.u. (8.66 Å). The outermost lattice plane of the ionic lattice which the background shown here represents is at $x = -\frac{1}{2}d$, with d the interplanar spacing (neglecting changes of spacing that may occur in the surface region). The outermost (111) plane of a semiinfinite fcc lattice, for example, would be at $x = -0.226Z^{1/3}$ Fermi wavelengths, the outermost (110) plane of a bcc lattice would be at $x = -0.219Z^{1/3}$ Fermi wavelengths, with Z the ionic charge. [$Z = 3$ for Al ($r_s \sim 2$), $Z = 1$ for K ($r_s \sim 5$), for example.]

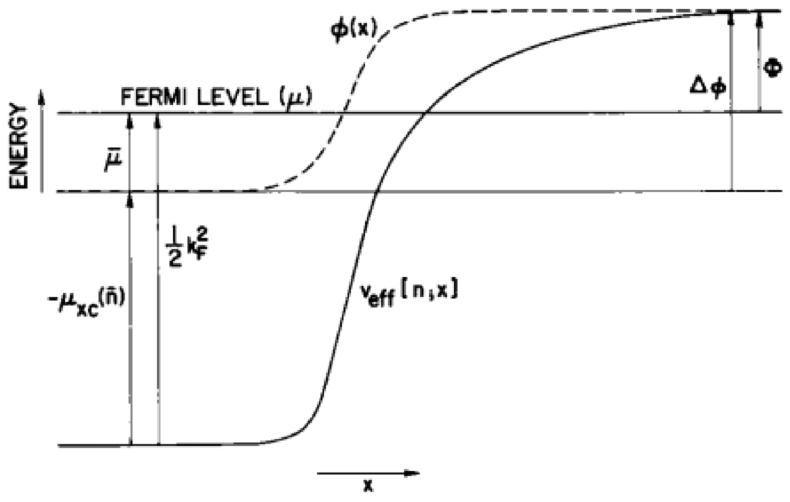


FIG. 3. Schematic representation of the potentials at a metal surface (planar uniform-background model). The bulk chemical potential $\bar{\mu}$ is shown here as positive, but it can have either sign (Table I).

Jellium model

N D Lang, Solid State Physics, v. 28, p. 225-300 (1973)

IMAGE FORCES: HIDDEN MANY-BODY PHENOMENA. SURFACE PLASMONS

Volume 38A, number 3 PHYSICS LETTERS 31 January 1972

SURFACE PLASMONS AND THE IMAGE FORCE IN METALS

R. H. RITCHIE

It is shown that the classical image potential acting between a point classical charge and a metal surface may be regarded as originating in the shifted zero point energy of the surface plasmon field. The retardation correction to the image potential is studied using the electron gas model.

The energy shift ΔE due to the charge Ze interaction with the surface plasmon field

$$\Delta E(x) = -\frac{(Ze)^2}{2c}\int_0^\infty \kappa\,\mathrm{d}\kappa \left\{\frac{\omega_\kappa}{p_\kappa}\left(\frac{1}{\nu_0}+\frac{1}{\nu}\right)^2\right\}\exp(-2\kappa x)$$

$$\epsilon(\omega) = \epsilon_1(\omega) + i\epsilon_2(\omega)$$

Temporal dispersion of the dielectric function

x is the distance of the charge from the vacuum-metal interface

For small x $\Delta E(x) = -(Ze)^2/4x$

IMAGE FORCES FOR MOVING CHARGES: TEMPORAL AND SPATIAL DISPERSION. SURFACE PLASMONS

PHYSICAL REVIEW B VOLUME 8, NUMBER 4 15 AUGUST 1973

J. Heinrichs **Response of Metal Surfaces to Static and Moving Point Charges and to Polarizable Charge Distributions**

$$W=\frac{q(t)}{4\pi}\int_{-\infty}^{\infty}d\omega\, e^{-i\omega t}\int_{0}^{\infty}dk_{\parallel}$$

$$\times\int_{-\infty}^{\infty}dt'\, e^{i\omega t'}q(t')\, e^{k_{\parallel}[z_0(t)+z_0(t')]}\,\frac{1-\epsilon_s(k_{\parallel},\omega)}{1+\epsilon_s(k_{\parallel},\omega)}\,,$$

$$z_0(t)<0 \qquad (4.16)$$

where

$$\epsilon_s(k_{\parallel},\omega)=\left[\frac{k_{\parallel}}{\pi}\int_{-\infty}^{\infty}\frac{dk_z}{k^2\epsilon(k,\omega)}\right]^{-1}. \qquad (4.17)$$

The account of both spatial and temporal dispersions leads to the saturation of image force energies at interfaces!

Damping of surface plasmons is essential since it eliminates the image force (polarization) energy oscillations far away form the interfaces!

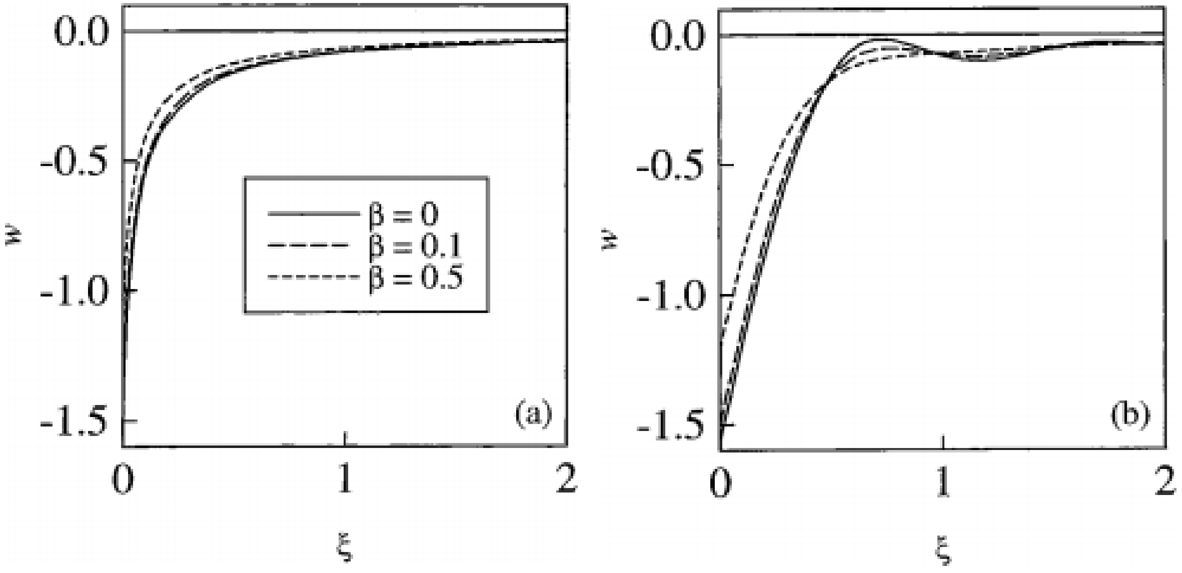
$$\epsilon(\omega)=1-\frac{\omega_p^2}{\omega(\omega+i\nu)}$$

$\omega_p=\omega_s\sqrt{2}$ is the bulk plasmon frequency and ν is the inverse relaxation time

phys. stat. sol. (b) **214**, 29 (1999) **Importance of the Plasmon Damping for the Dynamical Image Forces**

A. M. Gabovich, V. M. Rozenbaum, and A. I. Voitenko

IMAGE FORCES: TEMPORAL DISPERSION. MOVING CHARGES



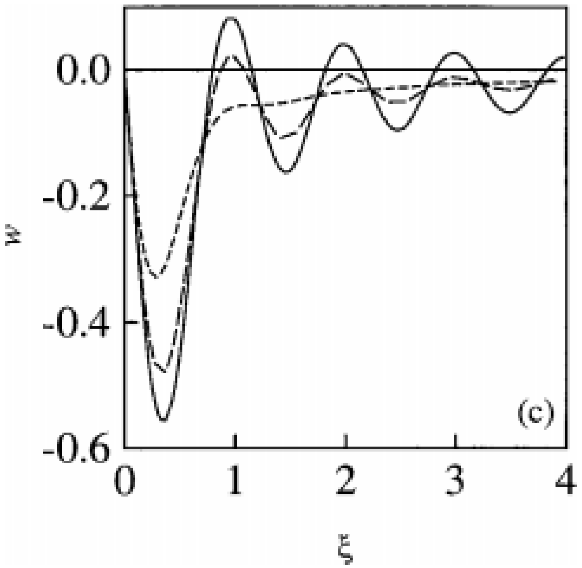


Fig. 1. Dependences of the dimensionless image force energy $w = 2vW/q^2\tilde{\omega}_s$ on the dimensionless distance $\xi = z/L$ reckoned from the metal surface into the vacuum for various values of the plasmon dissipative parameter $\beta = \nu/\omega_p$. Part a) corresponds to the normal motion of the charge q with the speed v from the infinity towards the surface, part b) corresponds to the same charge reflected from the surface, and part c) corresponds to the normal motion of the charge q with the speed v emitted from the surface. Here $L = 2\pi v/\tilde{\omega}_s$, $\tilde{\omega}_s = (\omega_p^2/2 - \nu^2/4)^{1/2}$ is the "softened" surface plasmon frequency, ω_p is the bulk plasmon frequency, ν is the inverse relaxation time of plasmons

Oscillations are due to real plasmon excitation

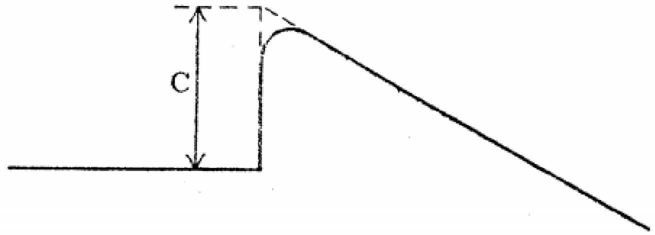
DYNAMICAL IMAGE FORCES: TUNNELING ELECTRONS IN FIELD EMISSION

R. H. Fowler; L. Nordheim **Electron Emission in Intense Electric Fields**

Proceedings of the Royal Society of London. Series A, Containing Papers of a Mathematical and Physical Character, Vol. 119, No. 781 (May 1, 1928), 173-181

$$j = CF^2 e^{-\alpha/F}$$

In the absence of image forces



$$j = \frac{m_e e}{2\pi^2 \hbar^3} \int_{-E_0}^{-\mu} dE\,(-\mu - E) D(E, F)$$

F is electrostatic field

$$D(E, F) = \exp(-I)$$

$$I = \frac{2}{\hbar} \int_{r_1}^{r_2} dr\,(2m_e |E + eFr - W(r)|)^{1/2} \quad W(0) = -\tfrac{1}{3} e^2 \kappa \left(1 + \tfrac{5}{16} e\kappa F/m\omega_p^2\right)$$

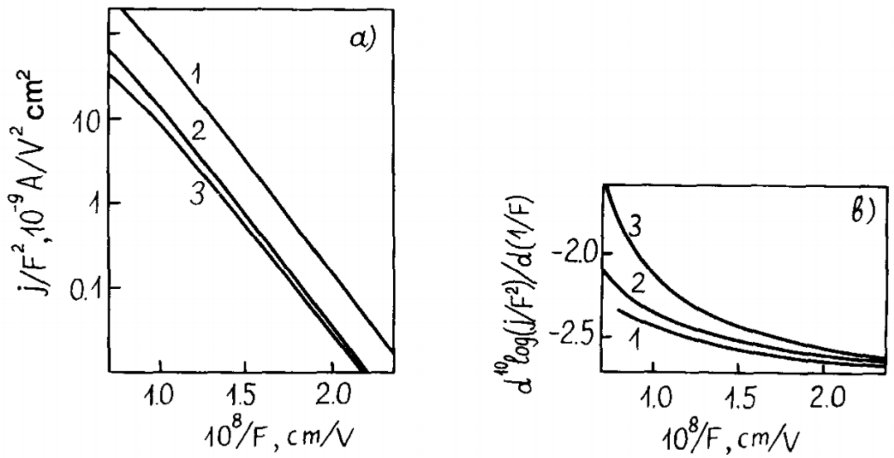


Fig. 2. (a) Current–voltage characteristics of the field-emission current from tungsten. Here j is the current density, and F is the electrostatic field. (b) Field dependence of the current–voltage characteristic slope. See notations in the text.

Curve 3 takes into account the dynamic field-dependent correction. It explains the observed deviations from the Fowler-Nordheim law.

A.M. GABOVICH, V.M. ROSENBAUM and A.I. VOITENKO

DYNAMICAL IMAGE FORCES IN THREE-LAYER SYSTEMS AND FIELD EMISSION

Surface Science 186 (1987) 523–549

IMAGE FORCES AND CHARGE-CHARGE INTERACTION: THREE-LAYER SYSTEMS. EXACT FORMULAS

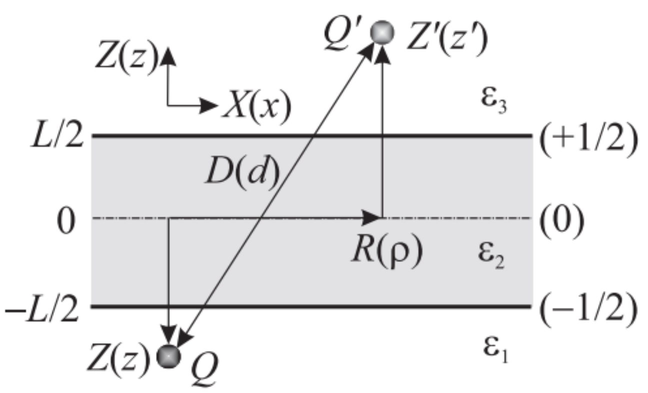


FIG. 1. Arrangement of the charges Q and Q' in a three-layer plane heterostructure. The width of interlayer 2 (slab) is L. Layers 1 and 3 (covers) are semi-infinite. ε_i ($i = 1, 2, 3$) are dielectric constants of the corresponding layers. Dimensional quantities are denoted by capital letters, dimensionless quantities normalized by L are denoted by lowercase letters and in parentheses. The coordinate Z (or z) is normal to the interfaces, and the coordinate X (or x) is parallel to them. The coordinate Z is reckoned from the middle of the interlayer. D (or d) is the distance between the charges, whereas R (or $\rho = R/L$) is the lateral distance between them.

$$W(Z, Z', R) = -2QQ' \int_0^\infty K\, dK\, D(K, Z, Z')J_0(KR)$$

The function D(K,Z,Z') is very cumbersome for three-layers and for specular reflection of charge carriers in each layer is expressed via following blocks

$$a_{1,3}(q, z) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{dk_\perp \cos k_\perp z}{(k_\perp^2 + q^2)\varepsilon_{1,3}(\mathbf{q}, k_\perp, \omega)}$$

$$a_{S,A}(q, z) = 2 \sum_{k_\perp^{S,A}} \frac{\exp\left[ik_\perp\left(z + \frac{1}{2}\right)\right]}{(k_\perp^2 + q^2)\varepsilon_2(\mathbf{q}, k_\perp, \omega)}$$

$$k_\perp^S = 2n\pi, \quad k_\perp^A = (2n + 1)\pi, \quad n = 0, \pm 1, \pm 2, \ldots .$$

A. M. Gabovich, M. S. Li, H. Szymczak, A. I. Voitenko,
Phys. Rev. B **105** (2022) 115415

In the general case, spatial and temporal dispersion are taken into account based on the Green's function method.

CHARGE IMAGE FORCES IN THREE-LAYER SYSTEMS: CLASSICAL ELECTROSTATICS

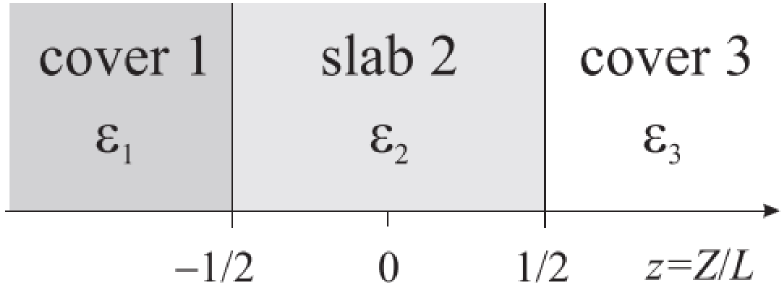


Figure 1. Scheme of the three-layer system: ε_i denote dielectric constants, L is the slab width, Z is the coordinate perpendicular to the layers, z is the reduced coordinate.

$$w = W\frac{L}{Q^2}, \qquad z = \frac{Z}{L}$$

$$w\left(z > \frac{1}{2}\right) = \frac{1}{4\varepsilon_3}\frac{\tau_{32}}{\left|z-\frac{1}{2}\right|} - \frac{\varepsilon_2\tau_{12}}{(\varepsilon_3+\varepsilon_2)^2}\Phi\left(-\theta, 1, \left|z+\frac{1}{2}\right|\right)$$

$$w\left(z < -\frac{1}{2}\right) = \frac{1}{4\varepsilon_1}\frac{\tau_{12}}{\left|z+\frac{1}{2}\right|} - \frac{\varepsilon_2\tau_{32}}{(\varepsilon_1+\varepsilon_2)^2}\Phi\left(-\theta, 1, \left|z-\frac{1}{2}\right|\right)$$

$$w\left(-\frac{1}{2} < z < \frac{1}{2}\right) = \frac{1}{4\varepsilon_2}\left[\tau_{21}\Phi\left(-\theta, 1, \left|\frac{1}{2}+z\right|\right) + \tau_{23}\Phi\left(-\theta, 1, \left|\frac{1}{2}-z\right|\right) - 2\ln(1+\theta)\right]$$

$$\tau_{ij} = \frac{\varepsilon_i - \varepsilon_j}{\varepsilon_i + \varepsilon_j} \qquad \theta = \tau_{12}\tau_{23}$$

$$\Phi(t, s, |z|) = \sum_{n=0}^{\infty}\frac{t^n}{(|z|+n)^s} = \frac{1}{\Gamma(s)}\int_0^{\infty}\frac{q^{s-1}\,\mathrm{e}^{-|z|q}}{1-t\,\mathrm{e}^{-q}}\mathrm{d}q,$$

is the Lerch transcendent

$$w(z=0) = \frac{1}{2\varepsilon_2}\left[\frac{(\varepsilon_2^2 - \varepsilon_1\varepsilon_3)}{(\varepsilon_2+\varepsilon_1)(\varepsilon_2+\varepsilon_3)}\Phi\left(-\theta, 1, \frac{1}{2}\right) - \ln(1+\theta)\right]$$

$$\Phi\left(-\theta, 1, \frac{1}{2}\right) = \begin{cases} \dfrac{1}{\sqrt{-\theta}}\ln\left|\dfrac{1+\sqrt{-\theta}}{1-\sqrt{-\theta}}\right| & \text{if } \theta < 0, \\ \dfrac{2}{\sqrt{\theta}}\arctan\sqrt{\theta} & \text{if } \theta > 0. \end{cases}$$

Exact results!

CHARGE IMAGE FORCES IN THREE-LAYER SYSTEMS: CLASSICAL ELECTROSTATICS

In the close vicinity of either interface, the interaction of the charge itself with the polarization charge induced at this interface strongly exceeds the interaction with the polarization charge induced at the other interface. Effectively, the problem also becomes two-layered even at $\varepsilon_1 \neq \varepsilon_2 \neq \varepsilon_3$, but in the short-distance limits. In particular, formulas (12) and (13) remain valid only asymptotically,

$$w\left(z \to \frac{1}{2} - 0\right) \to \frac{1}{4\varepsilon_2} \frac{\tau_{23}}{\left|z - \frac{1}{2}\right|}, \qquad (14)$$

$$w\left(z \to \frac{1}{2} + 0\right) \to \frac{1}{4\varepsilon_3} \frac{\tau_{32}}{\left|z - \frac{1}{2}\right|}. \qquad (15)$$

The problem symmetry brings about the same conclusion (with other constants) for the interface at $z = -\frac{1}{2}$.

The long-distance ($|z \to \infty|$) asymptotics of the $w(z)$ dependence deserve special consideration. In particular, if $\varepsilon_1 \neq \varepsilon_3$ and ε_2 is finite, it can be easily shown that in the depth of layer 3 ($z \to \infty$), the asymptotic limit of equation (9) is

$$w(z \to \infty) \to \frac{1}{4\varepsilon_3} \frac{\tau_{31}}{|z|}, \qquad (16)$$

i.e. the influence of the slab (ε_2) vanishes as if the interlayer disappears altogether. In this case, the long-distance asymptotics is equivalent to that in the two-layer configuration with a single interface between media 1 and 3 [cf equation (13)]. As a result of problem symmetry, we obtain a similar formula for the ($z \to -\infty$)-asymptotics,

$$w(z \to -\infty) \to \frac{1}{4\varepsilon_1} \frac{\tau_{13}}{|z|}. \qquad (17)$$

On the other hand, in the symmetric (s) case, when the sandwich covers are identical, we obtain $\tau_{31} = 0$, the expansion terms (16) and (17) vanish, and the next higher-order term in the long-distance expansion of, e.g., expression (9) has to be taken into account. It reads

$$-\frac{1}{4\varepsilon_3} \frac{2\varepsilon_3\left(\varepsilon_2^2 - \varepsilon_1^2\right) + \varepsilon_2\left(\varepsilon_1^2 - \varepsilon_3^2\right)}{2\varepsilon_2(\varepsilon_1 + \varepsilon_3)^2} \frac{1}{|z|^2}. \qquad (18)$$

Then, in the case $\varepsilon_1 = \varepsilon_3 = \varepsilon \neq \varepsilon_2$, the both long-distance asymptotics become identical and look like

$$w_s(z \to \pm\infty) \to \frac{\left(\varepsilon^2 - \varepsilon_2^2\right)}{16\varepsilon^2\varepsilon_2} \frac{1}{|z|^2}. \qquad (19)$$

So the image force energy turns out substantially weaker in comparison with the textbook behavior. It occurs because the polarization charges at both interfaces compensate each other in the first approximation. This fact was overlooked in the literature.

CHARGE IMAGE FORCES IN THREE-LAYER SYSTEMS: CLASSICAL ELECTROSTATICS

CREATION OF ELECTROSTATIC BARRIERS AND TRAPS FOR ELECTRONS OR IONS

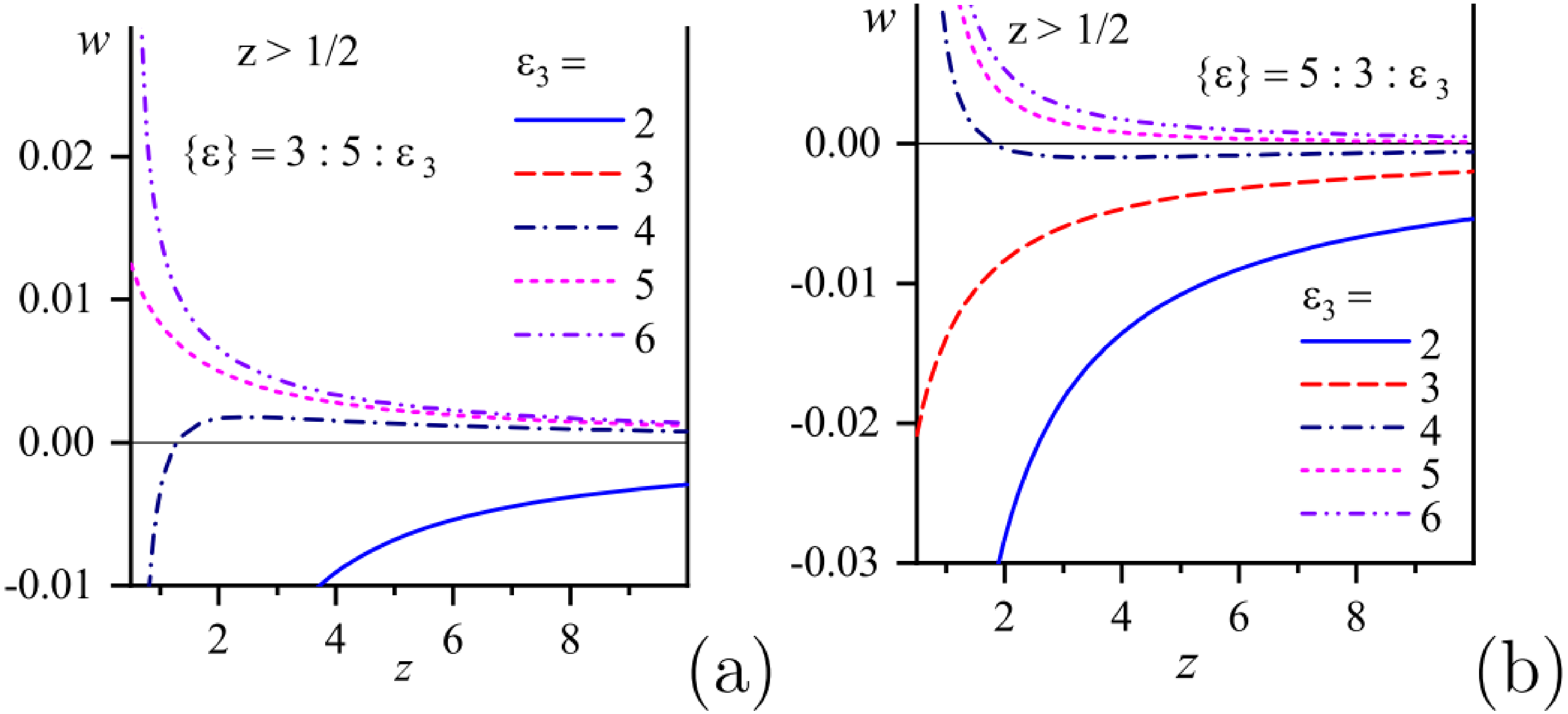


Figure 4. The $w(z)$-dependences in cover 3 for (a) $\{3 : 5 : \varepsilon_3\}$- and (b) $\{5 : 3 : \varepsilon_3\}$-structures with various ε_3's.

DIPOLE IMAGE FORCES IN THREE-LAYER SYSTEMS: CLASSICAL ELECTROSTATICS

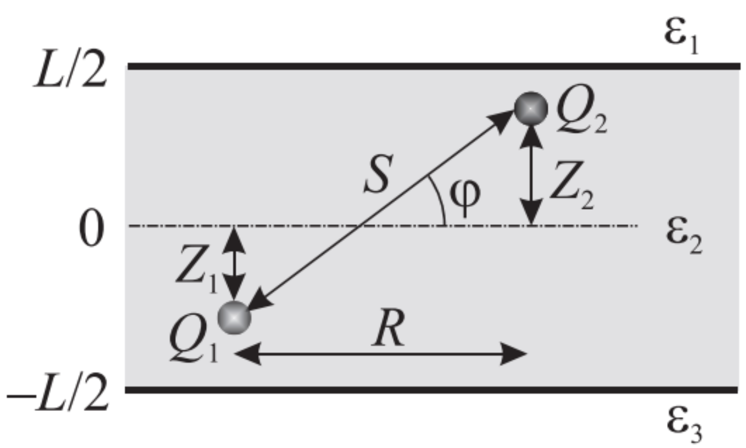
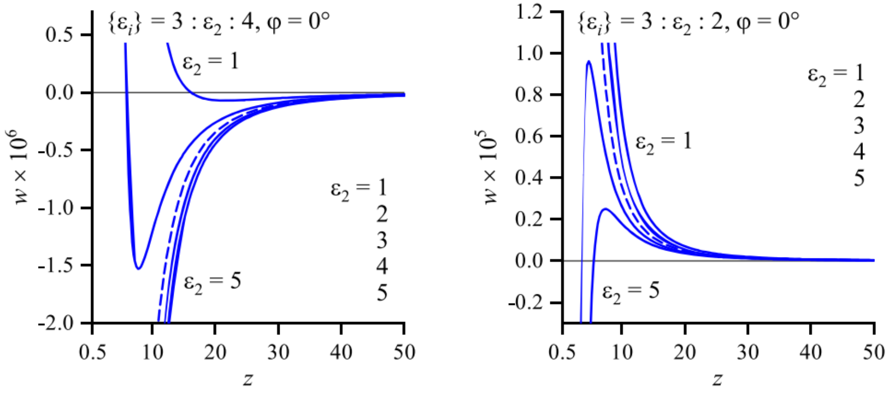


FIG. 1. A pair of interacting charges Q_1 and Q_2 located in a three-layer heterostructure with the constant dielectric permittivities of its layers $\{\varepsilon_i\} = \varepsilon_1 : \varepsilon_2 : \varepsilon_3$ at the coordinates Z_1 and Z_2, respectively, reckoned from the central plane $Z = 0$. The other parameters are as follows: S is the actual and R the lateral (along the interfaces) distance between the charges, φ is the orientation angle of the charge pair with respect to the interfaces, and L is the interlayer (medium 2) width.

$$w_2\left(-\tfrac{1}{2} < z < \tfrac{1}{2}\right) = \frac{(\varepsilon_1-\varepsilon_2)(\varepsilon_3-\varepsilon_2)\left(1-3\sin^2\varphi\right)\Phi(-\theta,1,3)}{8(\varepsilon_1+\varepsilon_2)\varepsilon_2(\varepsilon_2+\varepsilon_3)} + \frac{(\varepsilon_2-\varepsilon_3)\left(1+\sin^2\varphi\right)\Phi\left(-\theta,\tfrac{1}{2}+z,3\right)}{16\varepsilon_2(\varepsilon_2+\varepsilon_3)} + \frac{(\varepsilon_2-\varepsilon_1)\left(1+\sin^2\varphi\right)\Phi\left(-\theta,\tfrac{1}{2}-z,3\right)}{16(\varepsilon_1+\varepsilon_2)\varepsilon_2},$$

$$w_3\left(z < -\tfrac{1}{2}\right) = \frac{\left(1+\sin^2\varphi\right)}{16(\varepsilon_2+\varepsilon_3)} \times \left\{-\frac{(\varepsilon_3-\varepsilon_2)}{\varepsilon_3\left(z+\tfrac{1}{2}\right)^3} + \frac{4\varepsilon_2(\varepsilon_2-\varepsilon_1)\Phi\left(-\theta,\tfrac{1}{2}-z,3\right)}{(\varepsilon_1+\varepsilon_2)(\varepsilon_2+\varepsilon_3)}\right\}.$$



(a) (b)

For point dipoles both charges are located in the same layer!

$$w_1\left(z > \tfrac{1}{2}\right) = \frac{\left(1+\sin^2\varphi\right)}{16(\varepsilon_2+\varepsilon_1)} \times \left\{\frac{(\varepsilon_1-\varepsilon_2)}{\varepsilon_1\left(z-\tfrac{1}{2}\right)^3} + \frac{4\varepsilon_2(\varepsilon_2-\varepsilon_3)\Phi\left(-\theta,\tfrac{1}{2}+z,3\right)}{(\varepsilon_2+\varepsilon_3)(\varepsilon_2+\varepsilon_1)}\right\}$$

Reliability of the results: Extrema are located far from the interlayer

Formation of purely electrostatic traps and barriers for polar molecules.

CHARGE INTERACTION IN THREE-LAYER SYSTEMS: CLASSICAL ELECTROSTATICS

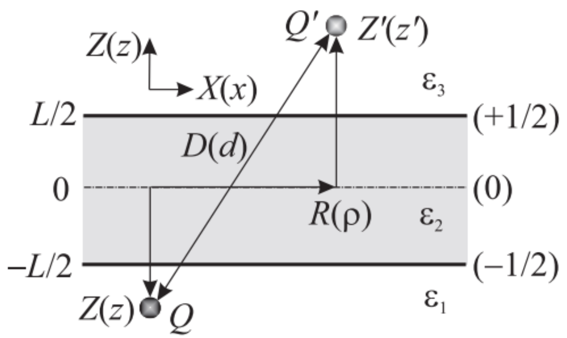


FIG. 1. Arrangement of the charges Q and Q' in a three-layer plane heterostructure. The width of interlayer 2 (slab) is L. Layers 1 and 3 (covers) are semi-infinite. ε_i ($i = 1, 2, 3$) are dielectric constants of the corresponding layers. Dimensional quantities are denoted by capital letters, dimensionless quantities normalized by L are denoted by lowercase letters and in parentheses. The coordinate Z (or z) is normal to the interfaces, and the coordinate X (or x) is parallel to them. The coordinate Z is reckoned from the middle of the interlayer. D (or d) is the distance between the charges, whereas R (or $\rho = R/L$) is the lateral distance between them.

The interaction energy *Wint* inside layers and for charge pairs from different layers are expressed in terms of

$$\Xi(\Lambda, \alpha, \rho) = \int_0^\infty \frac{\exp(-\alpha q)}{1 + \Lambda \exp(-2q)} J_0(\rho q) dq$$

$$\Lambda = \frac{(\varepsilon_1 - \varepsilon_2)(\varepsilon_2 - \varepsilon_3)}{(\varepsilon_1 + \varepsilon_2)(\varepsilon_2 + \varepsilon_3)}$$

J is the Bessel function

For ρ=0 all kinds of *Wint* are expressed analytically in terms of the Lerch transcendent.

Main problems, where one need to know the electrostatic interaction in three-layer systems:

1. Spectra of excitons in thin films
2. Spectra of interlayer excitons.
3. Excitonic insulators in three-layer systems.
4. Electron-hole superfluidity.

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Rytova-Keldysh approximation:

N. S. Rytova, Vestn. Mosk. Univ. **3**, 30 (1967) [arXiv:1806.00976]
L. V. Keldysh Journal of Experimental and Theoretical Physics Letters, Vol. 29, p.658 (1979)

As a rule, the formation of excitons in the slabs of three-layer systems is considered in the framework of the Rytova-Keldysh approximation (RKA) [1,32]. A detailed analysis of the latter was done in our work [33]. The RKA expression for the energy of charge-charge interaction in the case of symmetric structures ($\varepsilon_1 = \varepsilon_3 = \varepsilon$) and for $\varepsilon_2 \gg \varepsilon$ looks like (here, the variables are non-normalized, see Fig. 1)

$$W_{\mathrm{RKA}} = QQ' \frac{\pi}{\varepsilon_2 L}\left[\mathbf{H}_0\left(\frac{2\varepsilon}{\varepsilon_2}\frac{R}{L}\right) - N_0\left(\frac{2\varepsilon}{\varepsilon_2}\frac{R}{L}\right)\right], \qquad (32)$$

where $\mathbf{H}_0$ and N_0 are the Struve and Neumann functions of the zeroth order, respectively. Note that formula (32) does not include the Z coordinates of the charges. Its long-range ($R/L \to \infty$) asymptotics is identical to asymptotics (16). The RKA is very popular in relevant studies (see references in Ref. [33], as well as Refs. [37,144–148]). Although being derived for the conditions $\varepsilon \ll \varepsilon_2$, $R \gg L$, and $L \to 0$, it is sometimes overused when applying outside the indicated parameter region.

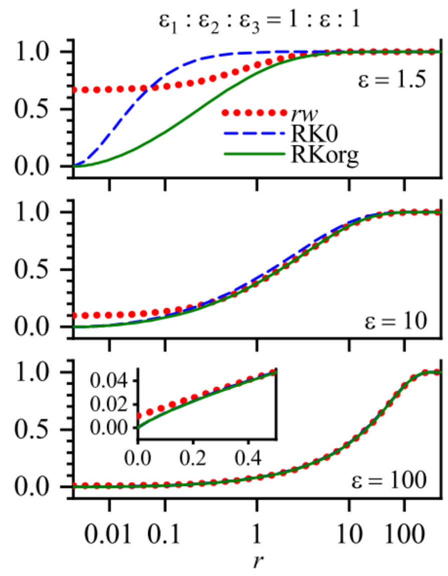

Figure 14. Dependences $rw(r)$ and the corresponding RK0 and RKorg approximations for symmetric structures D, F, and H. See explanations in the text.

Conclusion: RKA fails for conventional heterostructures with similar dielectric constants in different layers. For instance, ε = 13.1 and 10.1 for GaAs and AlAs, respectively.

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Effective-exponential approximations of the exact formulas

The function $\Xi(\Lambda, \alpha, \rho)$ was approximated and simple algebraic formulas obtained

$$\Xi(\Lambda, \alpha, \rho) \approx \frac{1}{\sqrt{\rho^2 + \alpha^2}} - \frac{\Lambda}{\Lambda + 1} \frac{1}{\sqrt{\rho^2 + (\alpha + a)^2}} \equiv \Xi_{\mathrm{EE}}(\Lambda, \alpha, \rho).$$

$$a_{\mathrm{EE1}} = \frac{2\Lambda}{(1 + \Lambda) \ln (1 + \Lambda)}$$

$$a_{\mathrm{EE2}} = \frac{2}{\Lambda + 1}$$

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Effective-exponential approximations of the exact formulas

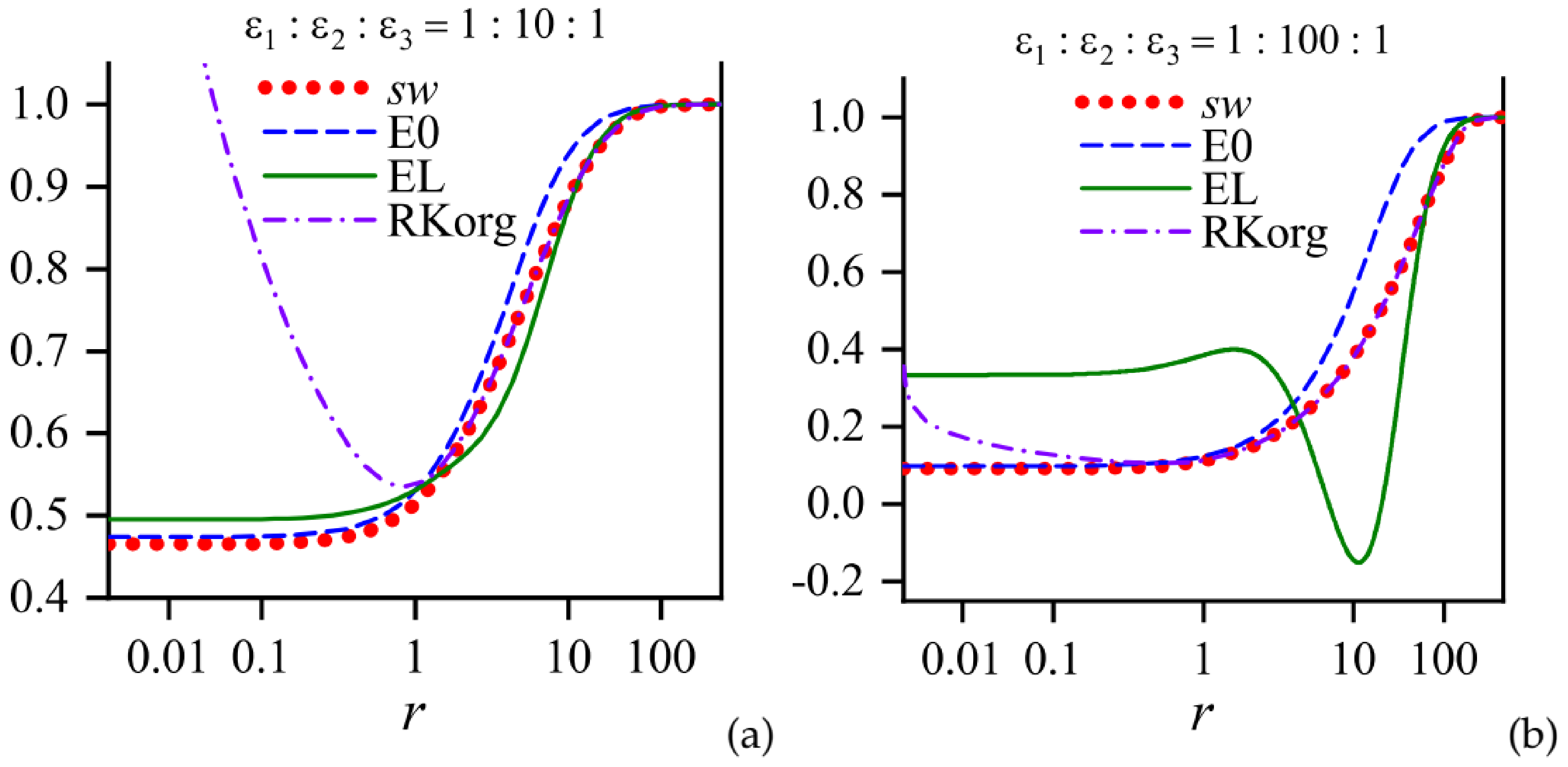

Figure 19. Dependence $sw(r)$ and its E0, EL, and RKorg approximations for symmetric structures: F (**a**); and H (**b**).

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For the “normal” arrangement of the charges ($\rho = 0$)

$$w_{33}(z,z',\rho=0) = \frac{1}{2\varepsilon_3}\left\{\Phi\left[-\Lambda,1,\frac{|z-z'|}{2}\right] + \Lambda\Phi\left[-\Lambda,1,\frac{|z-z'|+2}{2}\right] - \lambda_{12}\Phi\left[-\Lambda,1,\frac{|z+z'|+1}{2}\right] - \lambda_{23}\Phi\left[-\Lambda,1,\frac{|z+z'|-1}{2}\right]\right\},$$

$$w_{32}(z,z',\rho=0) = \frac{1}{(\varepsilon_2+\varepsilon_3)}\left\{\Phi\left[-\Lambda,1,\frac{|z-z'|}{2}\right] - \lambda_{12}\Phi\left[-\Lambda,1,\frac{|z+z'|+1}{2}\right]\right\},$$

$$w_{31}(z,z',\rho=0) = \frac{2\varepsilon_2}{(\varepsilon_1+\varepsilon_2)(\varepsilon_2+\varepsilon_3)}\left\{\Phi\left[-\Lambda,1,\frac{|z-z'|}{2}\right]\right\},$$

$$w_{11}(z,z',\rho=0) = \frac{1}{2\varepsilon_1}\left\{\Phi\left[-\Lambda,1,\frac{|z-z'|}{2}\right] + \Lambda\Phi\left[-\Lambda,1,\frac{|z-z'|+2}{2}\right] - \lambda_{32}\Phi\left[-\Lambda,1,\frac{|z+z'|+1}{2}\right] - \lambda_{21}\Phi\left[-\Lambda,1,\frac{|z+z'|-1}{2}\right]\right\},$$

$$w_{12}(z,z',\rho=0) = \frac{1}{(\varepsilon_2+\varepsilon_1)}\left\{\Phi\left[-\Lambda,1,\frac{|z-z'|}{2}\right] - \lambda_{32}\Phi\left[-\Lambda,1,\frac{|z+z'|+1}{2}\right]\right\},$$

$$w_{22}(z,z',\rho=0) = \frac{1}{2\varepsilon_2}\left\{\Phi\left[-\Lambda,1,\frac{|z-z'|}{2}\right] + \lambda_{21}\Phi\left[-\Lambda,1,\frac{1+(z+z')}{2}\right] + \lambda_{23}\Phi\left[-\Lambda,1,\frac{1-(z+z')}{2}\right] - \Lambda\Phi\left[-\Lambda,1,\frac{2-|z-z'|}{2}\right]\right\}.$$

Again, $w_{ji}(z,z',\rho=0) = w_{ij}(z,z',\rho=0)$.

GENERAL CONCLUSIONS:

1. Our original approach gives a practical scheme to calculate both polarization (image) forces and charge-charge or dipole-dipole-interaction in layered systems.

2. It is general enough to incorporate both temporal and spatial dielectric permittivities.

3. It allows to obtain exact analytical formulas in the classical electrostatic approximation.

4. It allows to obtain useful and relatively simple approximate formulas on the basis of cumbersome original expressions.

5. The results obtained have a large range of applicability in practically significant cases as inputs to solve a number of problems