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THEORY OF SYSTEMS WITH SMALL BOUNDARY ROUGHNESS IN APPLICATION TO ELECTRON STATES IN QUANTUM CHANNELS, ELECTRO- AND HYDRODYNAMICS

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The solutions of Laplace and wave equations in the systems with small one-dimensional surface roughness are studied. The conformal mapping technique is used. This permits the exact solution of Laplace equation and approximate solution of the wave one, if the characteristic height of the roughnesses is smaller then the wave-length. It is shown that such a rough boundary can be replaced by a flat one, however, shifted with regard to the mean surface position. This is correct, if the roughnesses are small, but maybe not smooth. Different physical problems at such boundary are reduced to this formulation. Namely, the effective capacity of a flat capacitor, the resistivity of a conducting layer, reflection of the electromagnetic wave on the metal surface, the laminar hydrodynamic flow in the rough 2D tube, the edge effects of the electron states in a quantum layer, the wave resistance of a planar waveguide.

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1. INTRODUCTION

In various fields of physics problems arise when it is necessary to solve the Laplace or wave equations

$$\begin{aligned} &\Delta\phi = 0 \quad \text{(Laplace)}, \\ &\Delta\psi + k^2\psi = 0 \quad \text{(wave)}. \end{aligned} \tag{1}$$

in domains with rough boundaries. In particular, such irregularities may be smaller than the characteristic spatial dimensions of the system. In this case the boundary can be replaced by some smooth one. The question arises where to put this smooth boundary. Although its position in zero approximation coincides with the averaged boundary, refining the position with the accuracy of the irregularity height requires solving the equations on the irregularity scale.

Generally speaking, any surface is rough at least on the atomic scale. However, semiconductor carriers have the wavelength larger than the lattice constant. The wavelength of light that interacts with matter is much longer. A small roughness is inevitable in such case. Nevertheless, the interaction with wave averages these roughness that makes the boundary electrically, hydrodynamically, optically or electronically smooth. However, the position of effective smooth boundary is determined by the solution of corresponding equations on the small distances, comparable with the roughness heights.

The problems of the parabolic equation solution in domains with a rough boundary arise in different fields of physics. The simplest ones are the problems of Laplace equation at such boundary.

For example, consider a plane capacitor with a rough surface. The problem is what is the capacitance of this capacitor with the accuracy of the inhomogeneity height? Similar problem arises when one wants to find the resistivity along a strip with a rough surface, or a laminar hydrodynamic flow in such a strip. In these cases, the problem converts to determination of the effective slab width.

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For a periodical rough boundary with height h and period l, the resulting effective border shift is $\alpha = hf(h/l)$, where the dimensionless function $f(x)$ is determined by a specific border shape. $f(0) = 0$ and $f(\infty) \sim 1$, if the border is counted from its mean position. Generally, the field direction significantly depends on the distance to the mean surface. Our purpose is to find the function $f(x)$. It is apparent, the quantity α is not equal to the mean surface height, due to screening of the metal tips by the underlying boundary dips.

A similar problem arises with the wave equation. If the boundary with zero condition for a tangential or normal field component has small (as compared with the wavelength) inhomogeneties, than they are negligible. However, the effective boundary position needs to be found, because it affects the solution phase. In the near-border domain with a width less than the wavelength, the wave equation is reduced to the Laplace one.

The present paper deals with the 2D wave equation. In this case the 2D Laplace equation can be exactly solved by the powerful conformal mapping methods [1].

In the papers [2–5] the electron scattering by the surface roughnesses in quantum films was considered. The models of these papers include the expansion on the powers of the irregularity height. In fact, as it is shown here, the smallness of slopes is also required. Indeed, on the scale of the irregularity height, smaller than the wavelength, the wave equation turns into the Laplace one. This equation has a more complected solution than that follows from the approximate boundary condition.

The light scattering in the systems with rough surfaces was the subject of multiple studies (see, for example, [6, 7]). The problem has been studied numerically in Ref. [8]. The papers [5, 9] consider the same problem for the small and mildly sloping roughnesses; however, the experiments [5] show that sharp sloping roughnesses can be also important. Unlike the theoretical studied cited before, here we focus attention to the small, but not mildly sloping roughnesses, where the light wave effectively smoothes out the rough boundary. As the result, the mean phase shift of the reflected wave occurs. Despite the small and mildly sloping roughnesses their contribution can not be considered as perturbation, because the roughness shape essentially change the wave field over the roughness height scale.

The rough surface capacitance was the subject of numerical study in the capacitance microscopy [10–12], and near-field microscopy [13, 14] microwave probes, which involve the capacitance between irregular conducting surfaces. However, no exact solution was found in that case.

Unlike [2], here we consider a purely two-dimensional problem not restricting ourselves by the gentle-slope-irregularities. The solution of the Laplace equation in vicinity of the rough surface can be obtained exactly for many types of irregularities in this case. This allows us further using the solution of the Laplace equation at the distances comparable to the irregularity size and then matching it with the solution of the Schrödinger equation at distances exceeding the irregularity height.

In the present paper, the Laplace equation in a 2D system with a rough but averagely flat boundary is solved using conformal mapping. This problem is reduced to an effective flat boundary shifted by some value from the average boundary.

This solution is extended to the wave equation, when the roughness is less than the wavelength, but can be sharp. The reflection phases are found for external scattering on a metal surface.

It should be emphasized that the zero condition on a boundary with a small (compared to the wavelength) roughness generates a change in the solution of the wave equation in the general region of their sizes, where the wave properties are negligibly small. The latter means a conversion of the wave equation to the Laplace equation in this region. The matching of the solutions of the Laplace and wave equations has been done using their asymptotics at the distances y from the boundary: $h \ll y \ll 1/k$.

The domain under study is shown in Fig. 1. Corrugated surface, where the zero boundary condition applied, can be replaced by an effective boundary shifted by some value α from the mean one. The main purpose of the paper is to find α for different boundary shapes.

Similar approach has been used in Ref. [15] where the conformal mappings were applied to the problem of surface plasmon scattering at the rough metal nanostructures. In this paper the roughnesses comprise array of the cylindric protrusion partly embedded in the

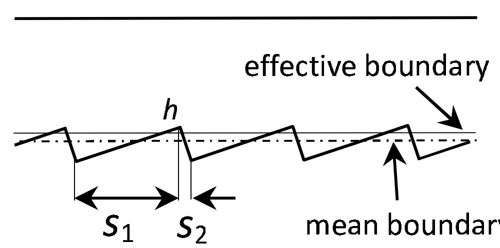

Fig. 1. Sketch of the system with toothed border under consideration

metal surface. The size of cylinders allows to reduce the wave equation to the Laplace one and then apply the conformal mapping.

2. PAPER STRUCTURE

We are based on the 2D Laplace equation $\Delta\phi = 0$ with the boundary condition $\phi = 0$. The boundary is assumed to be averagely straight, but uneven. Apart from this boundary ϕ behaves linearly as a function of the distance from this boundary. The shape of the boundary is the periodic broken line presented in Fig. 1. This shape permits exact solution, so that the effective shift of the boundary due to the roughness can be found.

Mathematically, the similar problem formulation arises in different fields of physics. In particular, in electrodynamics, fluid mechanics, physics of low-dimensional systems. Our aproach yields a way to find with accuracy of about the roughness height the following: 1) effective capacitance of plane capacitor with a rough electrode; 2) effective longitudinal conductance of a conductive strip; 3) to solve the hydrodynamic problem of laminar flow in a pipe with rough boundary and find the effective pipe width. The solution yields an effective shift of the boundary due to the roughness which can be expressed via an effective mixed boundary condition for the potential ϕ.

Different periodic broken-line boundaries can be considered in the same way. In particular, we find the effective boundary shift for the sawtooth boundary and the boundary with tips.

This problem formulation can be generalized to the solution of the wave equation $\Delta\phi + k^2\phi = 0$, for the small wave vector k. The wave equation is applicable to the electromagnetic wave reflection from a rough metallic surface. One can also apply a similar consideration to study the total internal reflection of light, if the dielectric constant of the medium is large. In addition, by means of these solutions, one can find the wave resistance of a plane waveguide. Also, the wave equation solution can be applied for electron states in a film or a 2D strip with a rough boundary.

We begin with the Laplace problem in a strip with the zero boundary conditions on the periodic broken line boundary. The problem is studied using conformal mapping of the domain with the rough boundary onto the halfplain. Then the solution for the boundary with sharp cuts has been obtained. After that we consider the generalization of the problem to the arbitrary broken line periodic boundary. These solutions are applied to find the effective width of the plane capacitor, resistivity of a strip, and the width of tube for laminar hydrodynamic flow. Then the reflection of the electromagnetic wave at the corresponding metallic surface has been found. After that the problem of shallow states in a semiconductor film with zero boundary conditions has been considered.

Then the electron motion along a strip with a boundary having a bump has been studied by the introduction of the effective potential caused by the conformal mapping. In the specific problem of a strip with a single cut this potential and the reflection coefficient where found.

3. LAPLACE PROBLEM IN A STRIP WITH ZERO BOUNDARY CONDITIONS ON A PERIODIC BROKEN-LINE BOUNDARY

Consider the solution of the Laplace equation at the metal boundary the shape of which is a periodic broken line presented in Fig. 1. The mapping of the upper half-plane onto the upper half-plane bounded by the broken line is given by the Christoffel-Schwarz integral (see, *e.g*, [1, 16, 17]):

$$w(z) = E_z \int dz (z+b)^{\beta} (z-b)^{-\beta} \times \\ \times \prod_{n=-\infty; n\neq 0}^{\infty} \left(1 - \frac{z+b}{na}\right)^{\beta} \left(1 - \frac{z-b}{na}\right)^{-\beta}. \quad (2)$$

Here $\pm\beta\pi$ are the inner and outer angles of the broken line, a is the line period, $\pm b$ are the images of vertices, n are integers, and E_z is a constant (we show further that it is the magnitude of the homogeneous field far from the boundary); all these parameters are real. The expression (2) can be transformed to the form

$$w(z) = E_z \int_0^z f(z) dz, \quad (3)$$

$$f(z) = \sin^{\beta}\left(\pi \frac{z+b}{a}\right) \sin^{-\beta}\left(\pi \frac{z-b}{a}\right),$$

and

$$s + ih = \int_{-b}^{b} dx (f(x) - 1), \\ s' - ih = \int_{b}^{a-b} dx (f(x) - 1), \quad (4)$$

where $a > b$. The quantity $s + s'$ determines the period in the plane w (s and s' can be of different signs).

4. PLANE CAPACITOR WITH ROUGH SURFACE

Consider the flat capacitor one plate of which is of the boken-line shape presented in Fig. 1. The potential is given by $\phi(z) = -\mathrm{Im}(w(z))$. Its asymptotics are $\phi(0) = 0$ and

$$\phi(z) \approx -E_z \left(y + \mathrm{Im} \int_0^{i\infty} dx\,(f(x) - 1) + ... \right)$$

at $z \to i\infty$. The heights h and widths s and s' of steps are determined by the relations (4). The case of a right-triangle boundary is specified by $\beta = 1/2$. This case describes, for example, a step-like surface of a vicinal face of a growing crystal, if $s' \ll s$. At $\beta = 1/2$ the integrals in expressions can be found exactly.

Eq.(5) connects the potential and field in the asymptotics with the shape of the teeth. Equation (5) can be rewritten as an effective boundary condition at $y = 0$, $\phi + \alpha \partial_y \phi = 0$, with

$$\alpha = \mathrm{Im} \int_0^{i\infty} (f(x) - 1)dx \qquad (5)$$

or $\phi(\alpha) = 0$.

The capacitance C of a capacitor increases due to a decrease in its thickness $C \to C(1 + \alpha/d)$. Another structure contains extremely thin tips, such as that shown in Fig. 2. The mapping of a half-plane onto a half-plane with cuts is given by the function

$$w = \frac{a}{\pi} \arccos \left(\frac{\cos\left({}^{\pi z}\!/_{a}\right)}{\mathrm{ch}\left({}^{\pi h}\!/_{a}\right)} \right) \qquad (6)$$

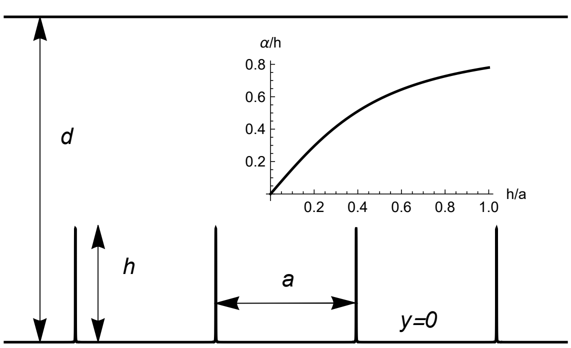

Fig. 2. Strip with periodically located extremely thin tips on the border. Insert: dependence of α/h vs a/d

The potential in the capacitor problem is given by its real part, and the electric field is determined by expression

$$E_x + iE_y = \frac{dw(z)}{dz}.$$

The constant α in the effective boundary condition is

$$\alpha = a \ln(\mathrm{ch}(\pi h/a))/\pi.$$

The limiting cases yield

$$\alpha \approx \pi h^2/a \quad \text{at} \quad \pi h \ll a, \qquad \alpha \approx h \quad \text{at} \quad \pi h \gg a. \qquad (7)$$

Equation (7) means that the influence of a sharp surface tip, on which the potential becomes zero, extends to the region of the order of the height of this tip. This is completely equivalent to the action of a lightning rod shielding objects located in such a region.

5. LIGHT REFLECTION BY A METAL SURFACE

Note that the solution to this problem of potential theory can be extended to the wave formulations, in particular, to the solution of the scalar wave (or Schrödinger) equation, if $kh \ll 1$. Here $k = 2\pi/\lambda$, h is the irregularity hight, and λ is the wavelength.

In the region close to the boundary by the distances $h \le |y| \ll \lambda$ the wave equation can be replaced with the Laplace one (see Fig. 3). While the effect of irregularity can be neglected at the distances $h \le y < \lambda$. This means that solutions of the wave and Laplace equations can be matched at $h \ll y \ll \lambda$.

Further we consider reflection of plane electromagnetic waves of two different polarisations: TE or **E**-wave, where $\mathbf{E} = (0, 0, E_z)$, $\mathbf{H} = (H_x, H_y, 0)$ and TH or **H**-wave, where $\mathbf{E} = (E_x, E_y, 0)$, $\mathbf{H} = (0, 0, H_z)$. It is apparent, the plane wave of arbitrary polarisation can be considered as linear combination of these ones.

Let the **E**-wave reflects from $y = +\infty$ at a rough metal surface $y \approx 0$ (case (a)). Then **E** obeys the equation $\Delta E_z + k^2 E_z = 0$ everywhere outside the metal. In vicinity of the surface $ky \ll 1$ we can neglect $k^2 E_z$ term in the wave equation and reduce it to the Laplace one $\Delta E_z = 0$.

The field E_z obeys the conditions $E_z = 0$ at the surface and $E_z = E_0 ky$ on the large distances ($h \ll y \ll 1/k$) from it. Hence, the complex field $E_z(u, v)$ conformally maps the upper vacuum plane

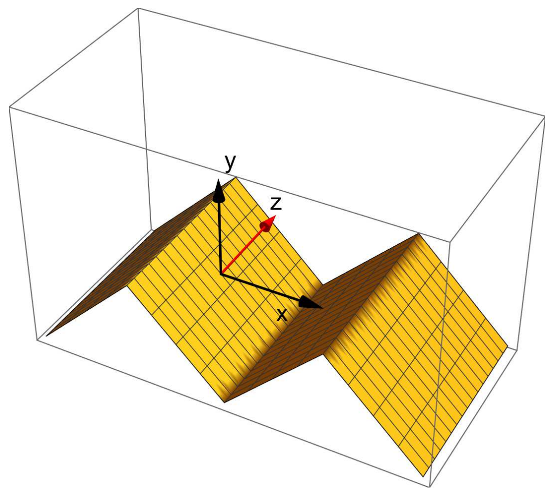

Fig. 3. Electromagnetic wave reflection from corrugated metal surface. The red arrow shows the direction of electric (case (a)) or magnetic (case (b)) fields

onto the halfplane $v > 0$. The result for the wave equation can be expressed via the boundary condition

$$E_z + \alpha \frac{dE_z}{dv} = 0$$

in the (u, v)-plane. The constant α is determined from solution of the Laplace equation.

Consider now incidence of the **H**-wave (case (b)). When the magnetic field **H** is directed along z-axes and obeys the boundary condition $\partial \mathbf{H}/\partial \mathbf{n} = 0$. Thus, H_z obey the wave equation $\Delta H_z + k^2 H_z = 0$ and the boundary condition $\partial H_z/\partial y = 0$. The problem can be reduced to the previous one by introducing the vector potential $\mathbf{A} = (A_x, 0, 0)$.

In Fig. 3 is shown the electromagnetic wave reflection from corrugated metal surface.

6. CONDUCTANCE OF A ROUGH STRIP

Consider the classical problem of conductance along a strip with conductivity σ and rough insulating boundaries. The solution of it is given by the equation for the current density $\mathbf{j}$

$$\nabla \mathbf{j} = 0, \quad \mathbf{j} = \sigma \nabla \varphi, \tag{8}$$

with the boundary condition $\mathbf{nj} = 0$, where $\mathbf{n}$ is the normal to the boundary. The total current in the sample along the surface is determined by the effective thickness. This problem is dual to the Laplace equation with boundary condition $\mathbf{n} \times \nabla \phi = 0$.

This solution is dual to the above considered capacitor problem. The effective strip width for corresponding geometries is reduced by the same quantity α found in the previous sections.

The same approach can be applied to the hydrodynamic problem of the laminar flow of liquid along the similar pipe. In this problems, the normal component of the fluid flow vanishes, that yields Eq.(8).

Note that in a rough waveguide the quantity α gives a decrease at the waveguide width thereby determining its wave impedance.

7. GENERALIZATION TO ARBITRARY PERIODIC BROKEN BOUNDARY

Let the boundary be a periodic broken line with vertices w_k, angles $\varphi_k = \pi(1 + \beta_k)$ and period a in the z-plane. Denoting the preimages of the vertices by b_n, instead of (2), we obtain

$$w(z) = E_z \int_0^z dz \prod_{k=1}^K \sin^{\beta_k}\left(\pi \frac{z - b_k}{a}\right), \tag{9}$$

where $\sum_k^K \beta_k = 0$ with conditions $w(b_k) = w_k$, which determine b_k. Instead of Eq.(4), we have

$$\alpha = \int_0^{i\infty} dz \left[\prod_{k=1}^K \sin^{\beta_k}\left(\pi \frac{z - b_k}{a}\right) - 1\right]. \tag{10}$$

8. ELECTRON REFLECTION BY TIP IN A STRIP

Next, we will consider the application of conformal mappings to solve the two-dimensional Schrödinger equation in a region with a rough boundary, not limiting ourselves by the smallness of the roughness height compared to the electron wavelength. This consideration is based on the fact that after transformation to curvilinear coordinates, an effective two-dimensional potential appears in the Schrödinger equation.

As an example, we will consider the reflection of electrons in a quantum 2D strip of width d from a single tip of height h (see Fig. 4).

We assume zero condition $\psi = 0$ on the strip and boundary. The conformal mapping converts the Schrödinger equation to

$$\Delta_w \psi + k^2 |dz/dw|^2 \psi = 0. \tag{11}$$

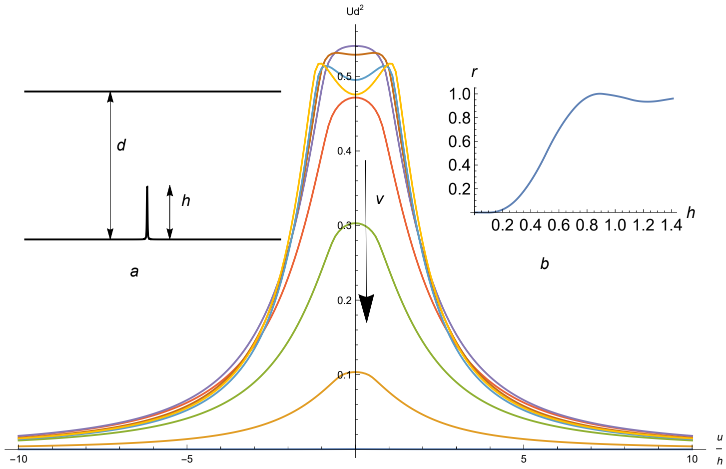

Fig. 4. Effective 1D potential in this strip *versus* u for different distances from the border. Inserts: strip with a single notch (*a*); reflection coefficient *versus* h in units of longitudinal wavelength (*b*). Arrow indicates growth of coordinate v

The knowledge of the conformal mapping $w(z)$ determines the effective potential $U(z)$ through the relation

$$2m(E - U(z)) \to k^2|dz/dw|^2. \tag{12}$$

Conformal mapping

$$w(z) = \frac{2d}{\pi}\times \times\left(\operatorname{arcth}\left(\cos\left(\frac{\pi h}{2d}\right)\sqrt{\operatorname{th}^2\left(\frac{\pi z}{2d}\right)+\operatorname{tg}^2\left(\frac{\pi h}{2d}\right)}\right)\right) \tag{13}$$

transforms a strip without a cut into a strip with a cut. If $(u, v, h) \ll d$, then the resulting potential is of the form in (Fig. 4 *b, c.*)

$$U(u,v) = \frac{k^2h^2}{\sqrt{4u^2v^2 + (u^2+v^2-h^2)^2}}. \tag{14}$$

The double-humped potential is explained by the fact that at the top the electron is farthest, on average, from the boundaries (most free), and at the corners it is closest to the boundary, that is, the potential is maximal. This dependence is inherited by the behavior of the potential in the plane w. At the points corresponding to the prototypes of the direct angles, the potential is maximal.

If $kh \ll 1$, the potential (14) can be replaced by the effective one-dimensional potential $U \to s\delta(u)$, where

$$s = \frac{2}{d}\iint \cos^2\left(\frac{\pi v}{d}\right)\frac{\pi^2h^2\,dudv}{d^2\sqrt{4u^2v^2+(u^2+v^2-h^2)^2}}.$$

The potential (insert *a*) as well as reflection coefficient (insert *b*) via corresponding barrier as a function of kh are presented in Fig. 4. Note the small nonmonotonicity of the curve in insert *b*. It is due to the double-humped character of the effective potential in the figure.

9. DISCUSSION AND CONCLUSIONS

We have considered problems from various fields of physics concerning the solution of the wave equation in a system with 1D rough boundaries. All the considered problems assume smallness of the roughness in comparison with the wavelength. This allows us to obtain a universal solution based on the conformal mappings theory. The result is the replacement of the rough boundary with an ideal one. The shift of it relative to the average boundary is $\alpha = bf(a/b)$; it is the function of the shape of the inhomogeneities, in particular, of their height h and width a. In contrast to the previously proposed approach with replacing the zero boundary condition with a mixed one $\psi + u(x,y)\partial_z\psi = 0$, the present approach is valid not only when $h \ll a$, but also when $h \sim a$. Despite the fact that the boundary shift is small, it significantly affects the quantization of particle states in size-quantized systems and light in Fabry-Perot resonators. The solution has been applied to determine the capacitance of a rough flat capacitor, the resistance of a two-dimensional conductor with a rough boundary, describing the laminar hydrodynamic flow in the corresponding pipe.

The problem of the phase of electromagnetic wave reflection from a metal surface was considered. We showed that the shift does not depend on the direction of light polarization.

The effective boundary condition we have found can be applied to determine the wave impedance of a waveguide, as well as the shift of the ground state of an electron in a quantum film or a strip.

Note that the solution of the Laplace equation by means of the conformal mapping can be applied to other low-dimensional structures, for example, to an intersection of quantum wires, when the Fermi wavelength is lower, than the wire width. We reserve this problem for future publications.

In the paper [8] the light refection from the dielectric surface with small roughness was considered by replacement of this surface with an effective 2D layer. In the simple analytical variant of consideration in [8] the spatially-dependent field (or induction) is approximated by their mean values. The exclusion is the numerical consideration in Supplement to [8]. The approach of the present paper is different: we base on the effective plane boundary shifted from the mean position. In our case all components of field present and essentially depend on coordinates. The conformal mapping permits find the field distribution analytically and obtain exact results for different shapes of surface. However, we are restricted by the case of reflection from metal only, which corresponds to infinite dielectric constant.

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