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Validity of the Rayleigh hypothesis for two-dimensional randomly rough metal surfaces

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Abstract. The Rayleigh hypothesis is the assumption that the field in the region above (below) a rough surface can be expressed as a weighted sum of upwards (downwards) propagating scattered (transmitted) modes, and that these expressions can be used to satisfy the boundary conditions on the fields at the surface. This hypothesis is expected to be valid for surfaces of sufficiently small slopes. For one-dimensional sinusoidal surfaces, the region of validity is known analytically, while for randomly rough surfaces in one and two dimensions, the limits of validity of the Rayleigh hypothesis are not known. In this paper, we perform a numerical study of the validity of the Rayleigh hypothesis for two-dimensionally rough metal and perfectly conducting surfaces by considering the conservation of energy. It is found for a perfect electric conductor that the region of validity is defined by the ratio of the root-mean-square roughness, δ, over the correlation length, a, being less than about 0.2, while for silver we find $\delta/a \lesssim 0.08$ for an incident wavelength $\lambda = 457.9$ nm. Limitations in our simulations made us unable to check the Rayleigh hypothesis for roughness where $\delta \gtrsim 0.13\lambda$.

1. Introduction

Randomly rough surfaces are abundant in nature and such structures may influence surface processes and phenomena in numerous ways. Lord Rayleigh is credited for being the first to study how wave scattering from surfaces is influenced by their roughness. In particular, at the end of the 19th century, he studied how waves are scattered by sinusoidal surfaces [1,2]. To this end, he assumed that the fields in the *surface region*, defined as the spatial region between the maximum and minimum points of the surface, can be written in a form similar to the asymptotic fields. This means that the reflected (transmitted) fields can be expressed as a weighted sum of upward (downward) propagating plane waves [see (4) and Ref. 3 for details].

This way of writing the fields in the surface region is an approximation which is expected to be valid if the surface structures have sufficiently small local slopes. Today this approximation is known as the *Rayleigh hypothesis* in honor of its inventor [1–4], and most perturbation theoretical treatments of the scattering problem can be constructed based on the assumption that the Rayleigh hypothesis is valid [3]. Moreover, by applying the Rayleigh hypothesis and imposing the boundary conditions satisfied by the fields at the surface, the so-called *reduced Rayleigh equation* for reflection (transmission) can be derived from the resulting coupled set of integral equations after eliminating the transmission (reflection) amplitudes [3,5]. The reduced Rayleigh equation, which contains either the unknown reflection or transmission amplitudes, has recently been solved by direct numerical means to produce non-perturbative results [3,6–8].

To take full advantage of an approximation, it is imperative to know its region of validity. About 75 years after its introduction, it was proven mathematically that the Rayleigh hypothesis for a sinusoidal surface[1], i.e., a surface which deviates from its mean by $x_3 = \zeta_0 \sin(\Lambda x_1)$, is formally valid if $\zeta_0 \Lambda \leq 0.448$ [9, 10]. However, for a randomly rough surface, the precise region of validity is still not formally known. For rough surfaces that are constant along one direction in the mean plane, i.e., their height can be written as $x_3 = \zeta(x_1)$, there have been attempts to use a direct numerical solution of the one-dimensional reduced Rayleigh equation to evaluate the validity of the Rayleigh hypothesis [11].

To the best of our knowledge, no attempt at a numerical study of the validity of the Rayleigh hypothesis has been reported in the literature for surfaces that are randomly rough along both directions of the mean plane. The lack of such a study in the literature is probably due to the significant computational cost. The purpose of this paper is to fill this gap in the literature by reporting some preliminary results for the validity of the Rayleigh hypothesis applied to electromagnetic wave scattering from two-dimensional randomly rough metal and perfectly conducting surfaces. Since this problem has no known analytic solution, we approach it by using a purely numerical solution of the reduced Rayleigh equation, which was recently implemented and tested [7].

For scattering from non-absorbing metallic substrates in vacuum, one must require that the power incident upon the surface equals the power reflected from it, since no energy can be transmitted through the metal. Hence, by numerically studying the conservation of energy in the simulated scattering process over the surface roughness parameter space, one may indirectly get information about the validity of the Rayleigh hypothesis which underlies the simulation approach being used. It should be stressed that the conservation of energy is a necessary, but not sufficient condition for correct results. Hence, the region of validity of the Rayleigh hypothesis for the systems we study here may in fact be even more restricted than what we report.

This paper is organized as follows: In Section 2, we define the geometry and some conventions used throughout the paper. Next, in Section 3, we describe the asymptotic field expansions, and write down the reduced Rayleigh equation for reflection from a perfectly conducting substrate, as well as the expression we will use to evaluate the conservation of energy, and we briefly describe how we proceed to solve the reduced Rayleigh equation. In Section 4, we present our results. We also include a discussion of these results, and what they can tell us about the limits on the validity of the Rayleigh hypothesis, as well as some discussion of other potentially limiting steps in our approach. Finally, we present some concluding remarks in Section 5.

2. Scattering geometry

The system we study consists of vacuum ($\varepsilon_1 = 1$) in the region $x_3 > \zeta\left(\boldsymbol{x}_\parallel\right)$, where $\boldsymbol{x}_\parallel = (x_1, x_2, 0)$ and a perfect electric conductor (PEC) or a metal in the region $x_3 < \zeta\left(\boldsymbol{x}_\parallel\right)$. The surface profile function $\zeta\left(\boldsymbol{x}_\parallel\right)$ is assumed to be a single-valued function of $\boldsymbol{x}_\parallel$ that is differentiable with respect to x_1 and x_2, and constitutes a zero-mean, stationary, isotropic, Gaussian random process defined by

$$\left\langle \zeta(\boldsymbol{x}_\parallel)\zeta(\boldsymbol{x}'_\parallel) \right\rangle = \delta^2 W\left(\left|\boldsymbol{x}_\parallel - \boldsymbol{x}'_\parallel\right|\right). \tag{1}$$

Here the angular brackets denote an average over the ensemble of realizations of the surface profile function. In writing (1), we have defined the root-mean-square height of the surface, $\delta = \left\langle \zeta^2(\boldsymbol{x}_\parallel) \right\rangle^{1/2}$, and $W(\boldsymbol{x}_\parallel - \boldsymbol{x}'_\parallel)$ is the height-height auto-correlation function of the surface,

[1] The coordinate system used is defined in Fig. 1.

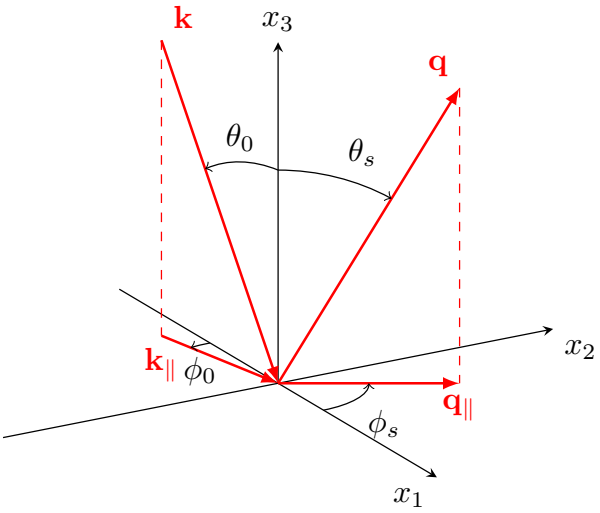

Figure 1. A sketch of the scattering geometry assumed in this work. The figure also shows the coordinate system used, angles of incidence (θ_0, ϕ_0) and scattering (θ_s, ϕ_s), and the corresponding lateral wavevectors $\boldsymbol{k}_\parallel$ and $\boldsymbol{q}_\parallel$, respectively.

normalized so that $W(\mathbf{0}) = 1$ [3]. The correlation function that will be considered in this work is isotropic and of the Gaussian form, given by

$$W\left(|\boldsymbol{x}_\parallel|\right) = \exp\left(-x_\parallel^2/a^2\right), \tag{2}$$

where a denotes the lateral correlation length.

3. Scattering theory

The electric field in the vacuum $\left[x_3 > \zeta\left(\boldsymbol{x}_\parallel\right)\right]$ is the sum of an incident field and a scattered field, $\boldsymbol{E}(\boldsymbol{x};t) = \left[\boldsymbol{E}(\boldsymbol{x}|\omega)_{\rm inc} + \boldsymbol{E}(\boldsymbol{x}|\omega)_{\rm sc}\right]\exp\left(-{\rm i}\omega t\right)$. The Rayleigh hypothesis consists of the assumption that the scattered field can be written as a weighted sum of upwards propagating modes, which allows us to write

$$\begin{aligned}
\boldsymbol{E}(\boldsymbol{x}|\omega)_{\rm inc} =& \left\{\frac{c}{\omega}\left[\hat{\boldsymbol{k}}_\parallel \alpha_1(k_\parallel) + \hat{\boldsymbol{x}}_3 k_\parallel\right] B_{\rm p}(\boldsymbol{k}_\parallel) + \left(\hat{\boldsymbol{x}}_3 \times \hat{\boldsymbol{k}}_\parallel\right) B_{\rm s}(\boldsymbol{k}_\parallel)\right\} \exp\left({\rm i}\boldsymbol{k}_\parallel \cdot \boldsymbol{x}_\parallel - {\rm i}\alpha_1(k_\parallel)x_3\right) \\
\boldsymbol{E}(\boldsymbol{x}|\omega)_{\rm sc} =& \int \frac{{\rm d}^2 q_\parallel}{(2\pi)^2}\left\{\frac{c}{\omega}\left[\hat{\boldsymbol{q}}_\parallel \alpha_1(q_\parallel) - \hat{\boldsymbol{x}}_3 q_\parallel\right] A_{\rm p}(\boldsymbol{q}_\parallel) + \left(\hat{\boldsymbol{x}}_3 \times \hat{\boldsymbol{q}}_\parallel\right) A_{\rm s}(\boldsymbol{q}_\parallel)\right\} \\
& \times \exp\left({\rm i}\boldsymbol{q}_\parallel \cdot \boldsymbol{x}_\parallel + {\rm i}\alpha_1(q_\parallel)x_3\right).
\end{aligned} \tag{3}$$

Here the subscripts p and s denote the p-polarized and s-polarized components of these fields with respect to the local planes of incidence and scattering. The expressions in front of the amplitudes $A_{\rm p}$ and $B_{\rm p}$ are the unit polarization vectors for p polarized light, and similarly the expressions in front of the amplitudes $A_{\rm s}$ and $B_{\rm s}$ are the unit polarization vectors for s polarized light. A caret over a vector indicates that it is a unit vector. The third component of the wave vector $\boldsymbol{q}$ in vacuum, $\alpha_1(q_\parallel)$, is given by

$$\alpha_1(q_\parallel) = \left[\left(\frac{\omega}{c}\right)^2 - q_\parallel^2\right]^{1/2}, \qquad {\rm Re}\,\alpha_1(q_\parallel) > 0,\ {\rm Im}\,\alpha_1(q_\parallel) > 0. \tag{4}$$

We assume that a linear relation exists between the amplitudes $A_\alpha(\boldsymbol{q}_\parallel)$ and $B_\beta(\boldsymbol{k}_\parallel)$ ($\alpha, \beta = \mathrm{p}, \mathrm{s}$), which we write as

$$A_\alpha(\boldsymbol{q}_\parallel) = \sum_\beta R_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) B_\beta(\boldsymbol{k}_\parallel).$$

It then can be shown that the scattering amplitudes, organized into the following 2×2 matrix

$$\boldsymbol{R}(\boldsymbol{q}_\parallel|\boldsymbol{x}_\parallel) = \begin{pmatrix} R_{\mathrm{pp}}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) & R_{\mathrm{ps}}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) \\ R_{\mathrm{sp}}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) & R_{\mathrm{ss}}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) \end{pmatrix}, \tag{5}$$

satisfy the matrix integral equation [12]

$$\int \frac{\mathrm{d}^2 q_\parallel}{(2\pi)^2} \boldsymbol{M}^+(\boldsymbol{p}_\parallel|\boldsymbol{q}_\parallel) \boldsymbol{R}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) = -\boldsymbol{M}^-(\boldsymbol{p}_\parallel|\boldsymbol{k}_\parallel). \tag{6a}$$

This equation is known as the *reduced* Rayleigh equation since it is an equation for the scattered field in the medium of incidence only. The elements of the matrices $\boldsymbol{M}^\pm$ for a perfect electric conductor take the form

$$\boldsymbol{M}^\pm(\boldsymbol{p}_\parallel|\boldsymbol{q}_\parallel) = I(\pm\alpha_1(q_\parallel)|\boldsymbol{p}_\parallel - \boldsymbol{q}_\parallel) \begin{pmatrix} \pm\frac{c}{\omega}\frac{p_\parallel q_\parallel - (\omega/c)^2\, \hat{\boldsymbol{p}}_\parallel \cdot \hat{\boldsymbol{q}}_\parallel}{\alpha_1(q_\parallel)} & [\hat{\boldsymbol{p}}_\parallel \times \hat{\boldsymbol{q}}_\parallel]_3 \\ \pm\frac{\omega}{c}\frac{[\hat{\boldsymbol{p}}_\parallel \times \hat{\boldsymbol{q}}_\parallel]_3}{\alpha_1(q_\parallel)} & \hat{\boldsymbol{p}}_\parallel \cdot \hat{\boldsymbol{q}}_\parallel \end{pmatrix}, \tag{6b}$$

where

$$I\left(\gamma|\boldsymbol{Q}_\parallel\right) = \int \mathrm{d}^2 x_\parallel \, \exp\left(-\mathrm{i}\boldsymbol{Q}_\parallel \cdot \boldsymbol{x}_\parallel\right) \exp\left[-\mathrm{i}\gamma\zeta\left(\boldsymbol{x}_\parallel\right)\right]. \tag{6c}$$

For a penetrable metal or dielectric surface, the corresponding matrix elements are given explicitly in Ref. 7, and will not be repeated here.

3.1. Mean Differential Reflection Coefficient

The solution of the reduced Rayleigh equation determines the scattering amplitudes $R_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$, where α and β signify the polarization of the reflected and incident light, respectively. When the incident field is known, this quantity completely specifies the scattered field in the region above the maximum point of the surface. However, $R_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ is not directly measurable in experiments. A more useful quantity is the mean differential reflection coefficient (DRC), which is defined as the fraction of the time-averaged incident power which is scattered by the surface into the solid angle $\mathrm{d}\Omega_s$ about the scattering direction $\boldsymbol{q}$ defined by the angles of scattering (θ_s, ϕ_s) (see Fig. 1). The mean DRC is defined as [13]

$$\left\langle \frac{\partial R_{\alpha\beta}}{\partial \Omega_s} \right\rangle = \frac{1}{L^2} \frac{\omega^2}{4\pi^2 c^2} \frac{\cos^2\theta_s}{\cos\theta_0} \left\langle \left| R_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel) \right|^2 \right\rangle, \tag{7}$$

where L^2 is the area of the plane $x_3 = 0$ covered by the rough surface, and θ_0 is the angle of incidence (see Fig. 1).

3.2. Conservation of Energy

To test whether the Rayleigh hypothesis is fulfilled, we use the conservation of energy as a criterion. Considering a perfectly conducting substrate, all the incident power must be reflected, and we can check whether our calculations conserve energy from the reflected field alone. The fraction of the time-averaged incident power in the form of light of polarization β, scattered by the surface into light of polarization α, is given by the integral of the corresponding mean DRC over the upper hemisphere:

$$\mathcal{U}_{\alpha\beta} = \int \mathrm{d}\Omega_s \left\langle \frac{\partial R_{\alpha\beta}}{\partial \Omega_s} \right\rangle. \tag{8}$$

If the substrate is non-absorbing, and the incident light has polarization β, one should have

$$\mathcal{U}_\beta = \sum_\alpha \mathcal{U}_{\alpha\beta} = 1, \tag{9}$$

since energy is conserved in the scattering process. To improve statistics, we define the quantity

$$\mathcal{U} = \frac{\mathcal{U}_\mathrm{p} + \mathcal{U}_\mathrm{s}}{2}, \tag{10}$$

which we find by separately calculating both $\mathcal{U}_\mathrm{p}$ and $\mathcal{U}_\mathrm{s}$ for each surface realisation, and taking their average. This is the quantity we will use when testing the validity of the Rayleigh hypothesis.

While the conservation of energy is a necessary, but not sufficient, condition for correct results, we have previously made successful direct comparisons of results obtained by the numerical solution of the reduced Rayleigh equation for weakly rough surfaces against both experimental data, and simulation results obtained by the rigorous surface integral method [14–16]. We are thus confident that our approach works well for weakly rough surfaces. Furthermore, if we hold the transverse correlation length of the surface roughness fixed, while increasing the rms height of the surface, we typically see that at some point, $\mathcal{U}$ starts increasing past 1. While $\mathcal{U} > 1$ is clearly unphysical, and thus evidence that the technique is not working, $\mathcal{U} = 1$ is not by itself proof that the results are correct (for a non-absorbing substrate). Still, our comparisons with both experimental data and other numerical data indicate that the conservation of energy is a useful guide to the validity of our approach.

Thus, in this paper we use $\mathcal{U} \approx 1$ as a criterion for when our approach is valid when considering a perfect electric conductor, and $\mathcal{U} \lesssim 1$ when considering a penetrable metal. Note that this criterion does not directly test the Rayleigh hypothesis, but rather our complete method for solving the scattering problem, which among other things relies on the Rayleigh hypothesis. There could be other reasons why our approach fails for strongly rough surfaces, and this will be discussed in more detail when considering our results.

3.3. Solving the reduced Rayleigh equation

To solve the reduced Rayleigh equation, we begin by numerically generating a realization of the surface profile function on a grid of N_x^2 points within a square region of the x_1x_2 plane of edge L, so that the in-plane sampling interval is $\Delta x = L/N_x$. A two-dimensional version of the filtering method used in Refs. [7, 16, 17] is used to generate the surface realizations from a given correlation function.

The next step is to evaluate the integrals $I(\gamma|\boldsymbol{Q}_\parallel)$ defined in (6c). These integrals are so-called Fourier integrals and care should be taken when evaluating them due to the oscillating integrands [18]. Using direct numerical integration routines for their evaluation will typically result in inaccurate results. Instead, a (fast) Fourier transform technique with end point

corrections may be adapted for their evaluation (the details of the method is outlined in Ref. [18]). However, these calculations are time consuming. In solving for $\boldsymbol{R}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$, we will discretize both $\boldsymbol{p}_\parallel$, $\boldsymbol{q}_\parallel$ and $\boldsymbol{k}_\parallel$, and $I(\gamma|\boldsymbol{Q}_\parallel)$ must be evaluated for all relevant combinations of the arguments $\gamma = \pm\alpha_1(p_\parallel)$ and $\boldsymbol{Q}_\parallel = \boldsymbol{p}_\parallel - \boldsymbol{q}_\parallel$ and $\boldsymbol{Q}_\parallel = \boldsymbol{p}_\parallel - \boldsymbol{k}_\parallel$. For the calculations used to generate the results presented in this paper, this would amount to evaluating $I(\gamma|\boldsymbol{Q}_\parallel)$ on the order of 10^9 times per surface realization.

A computationally more efficient way of evaluating $I(\gamma|\boldsymbol{Q}_\parallel)$ is to assume that the exponential function $\exp\left[-\mathrm{i}\gamma\zeta(\boldsymbol{x}_\parallel)\right]$, present in the definition of $I(\gamma|\boldsymbol{Q}_\parallel)$, can be expanded in powers of its argument, and then evaluating the resulting expression term-by-term by employing the Fourier transform. This gives

$$I(\gamma|\boldsymbol{Q}_\parallel) = \sum_{n=0}^{\infty} \frac{(-\mathrm{i}\gamma)^n}{n!} \tilde{\zeta}^{(n)}(\boldsymbol{Q}_\parallel), \tag{11a}$$

where $\tilde{\zeta}^{(n)}(\boldsymbol{Q}_\parallel)$ denotes the Fourier transform of the nth power of the surface profile function, i.e.,

$$\tilde{\zeta}^{(n)}(\boldsymbol{Q}_\parallel) = \int \mathrm{d}^2 x_\parallel \zeta^n(\boldsymbol{x}_\parallel) \exp\left(-\mathrm{i}\boldsymbol{Q}_\parallel \cdot \boldsymbol{x}_\parallel\right). \tag{11b}$$

In practice, the sum in (11a) will be truncated at a finite value of n. The Fourier transforms are calculated using a fast Fourier transform (FFT) algorithm.

The primary advantage of using Eqs. (11) for calculating $I(\gamma|\boldsymbol{Q}_\parallel)$ is that the rewrite in (11a) moves γ outside the integral, and calculating the integral in (11b) by FFT gives us the value of the integral as a function of $\boldsymbol{Q}_\parallel$. By using the proper discretization, we can make sure that the values of $\boldsymbol{Q}_\parallel$ resolved by the FFT are precisely those we need when setting up a linear equation system to solve for $R_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$. This alternative way of evaluating the I-integrals results in a significant reduction in computational time. The same method has previously been applied successfully to the numerical solution of the one-dimensional reduced Rayleigh equation [6,19,20].

It should be noted that the series expansion used to arrive at (11a) requires $\left|\gamma\zeta(\boldsymbol{x}_\parallel)\right| \ll 1$ to converge reasonably fast. Even though the series expansion of the exponential function is always convergent in theory, this procedure might not be numerically stable for large values of $\left|\gamma\zeta(\boldsymbol{x}_\parallel)\right|$, in particular due to the oscillatory nature of the series. Thus, limited numerical precision means that using the expansion presented in (11a) places additional constraints on the amplitude of the surface roughness which may be more restrictive than those introduced by the Rayleigh hypothesis. In particular, the Rayleigh hypothesis places a constraint on the maximum *slope* of the surface roughness, while the numerical procedure used to evaluate the I-integrals, needed to solve the reduced Rayleigh equation, also limits the *amplitude* of the surface roughness. Hence, surfaces exist for which the Rayleigh hypothesis is satisfied, but the above expansion method will not converge numerically, and the much more time-consuming approach of Ref. 18 will have to be applied.

Finally, in evaluating the integral in (6a) over $\boldsymbol{q}_\parallel$, the integration limits were truncated to the circular region defined by $\left(q_1^2 + q_2^2\right)^{1/2} \leq Q/2$. The Nyquist sampling theorem requires that $|q_1|$ and $|q_2|$ be smaller than $Q_c = \pi/\Delta x$ [21, p. 605]. The components of the vector $\boldsymbol{p}_\parallel - \boldsymbol{q}_\parallel$ entering $I(\gamma|\boldsymbol{p}_\parallel - \boldsymbol{q}_\parallel)$ lie in the interval $[-Q, Q]$, so we have chosen $Q = Q_c$. A quadratic grid with grid constant $\Delta q = 2\pi/L$ was constructed within the circular region of the q_1q_2 plane where $\left(q_1^2 + q_2^2\right)^{1/2} \leq Q/2$. The integral over this region in (6a) was carried out by a two-dimensional version of the extended midpoint method [21, p. 161] and the values of $R_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ were calculated for values of $\boldsymbol{q}_\parallel$ on the grid for a given value of $\boldsymbol{k}_\parallel$ (or equivalently, a given angle of incidence), which was also a point on the grid. The resulting matrix equations were solved

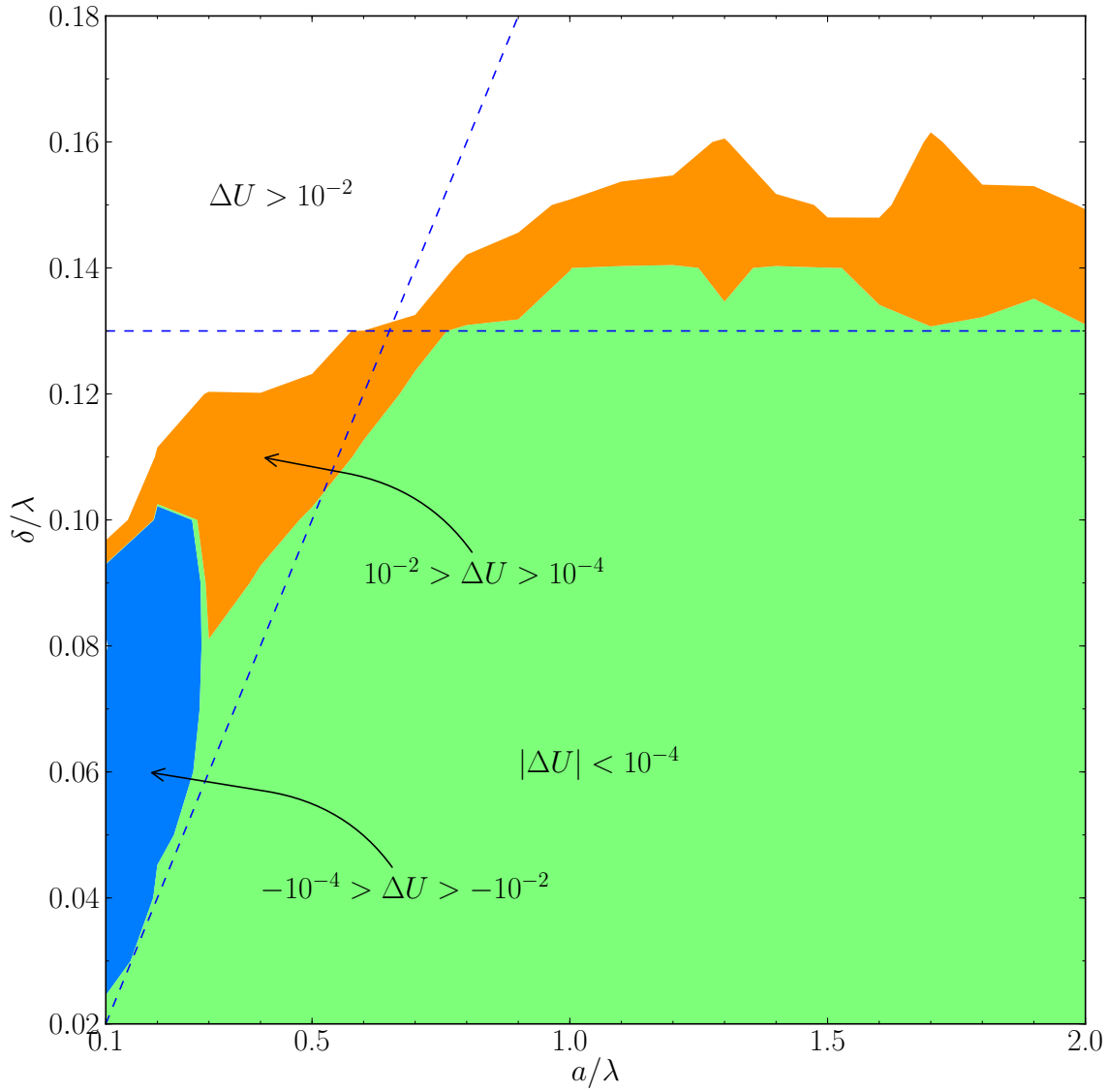

Figure 2. Contour plot of $\Delta\mathcal{U} \equiv \mathcal{U} - 1$, i.e., the deviation from unity of the fraction of incident power reflected from randomly rough surfaces on perfectly conducting substrates. The surface roughness is characterized by the correlation function given in (2), with the correlation length, a, given on the horizontal axis and the rms height of the surface, δ, on the vertical axis. The slope of the diagonal dashed line is given by $\delta/a = 0.2$, which corresponds to an rms slope of the rough surface of 0.28.

by LU decomposition and back substitution [21, p. 48]. In this way we obtain $R_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$, from which the mean DRC can be calculated [see (7)]. For a more detailed description of how we solve the reduced Rayleigh equation, we refer the interested reader to Ref. 7.

4. Results

The direct numerical solution method of the reduced Rayleigh equation from Sec. 3 has been used to calculate the scattering amplitudes $R_{\alpha\beta}(\boldsymbol{q}_\parallel|\boldsymbol{k}_\parallel)$ for randomly rough surfaces of edges $L \times L$, where $L = 15\lambda$. The surface profile function $\zeta(\boldsymbol{x}_\parallel)$ was discretized to $N_x \times N_x$ points, with

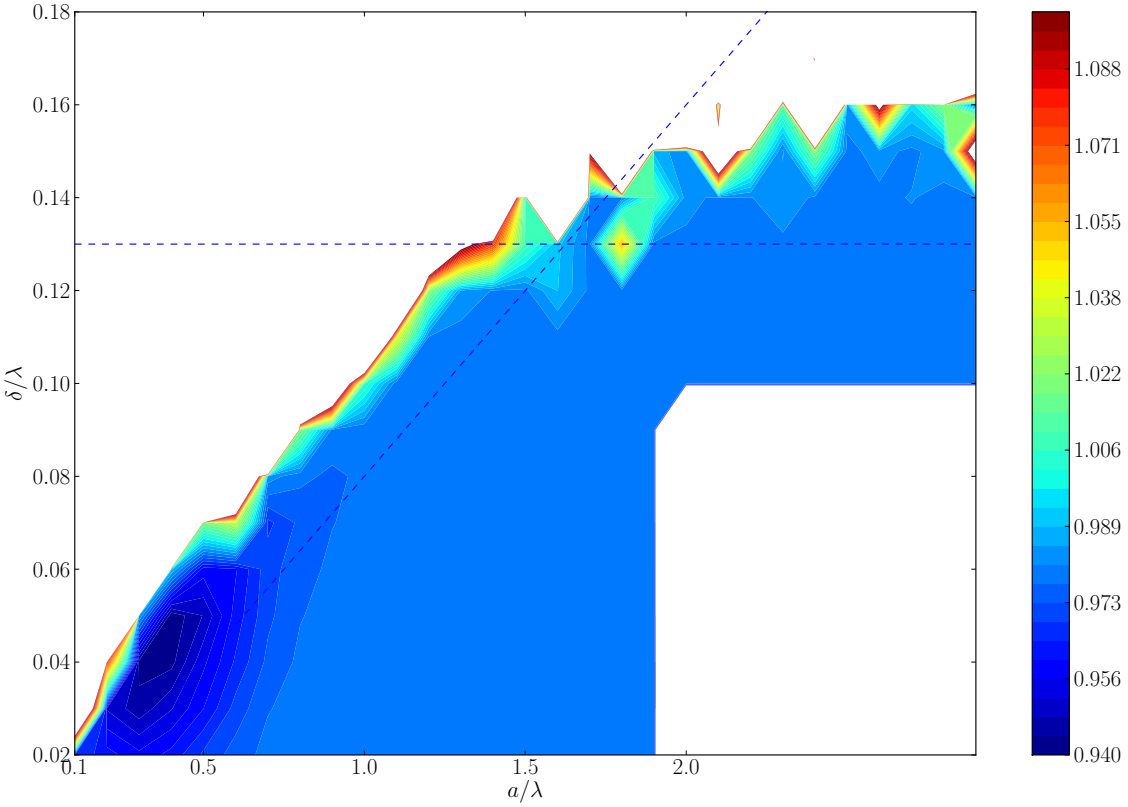

Figure 3. Contour plot of $\mathcal{U}$, the fraction of incident power reflected from randomly rough surfaces on silver substrates. The incident wavelength is 457.9 nm, which corresponds to a dielectric constant of $\epsilon_2 = -7.5 + 0.24\mathrm{i}$. The surface roughness is characterized by the correlation function given in (2), with the correlation length, a, given on the horizontal axis and the rms height, δ, on the vertical axis. The white area in the bottom right corner represents parameters for which we have no data, but where we are confident the value of $\mathcal{U}$ is the same as in the surrounding region. The white area in the upper left represents values of $\mathcal{U}$ greater than 1.1. The slope of the diagonal dashed line is given by $\delta/a = 0.08$, which corresponds to an rms slope of the rough surface of 0.11.

$N_x = 319$, and the roughness was characterized by the height-height autocorrelation function given by (2). The sum in (11a) was truncated at $n = 20$. Solving the reduced Rayleigh equation for one surface realization with these parameters takes approximately 17 minutes on a machine with two six-core AMD Opteron 2.1 GHz processors. The majority (around 90%) of this time is spent performing the LU-decomposition of the linear equation system.

The first set of results we present is for a perfectly conducting substrate. For this system, Fig. 2 depicts a contour plot of $\Delta\mathcal{U} \equiv \mathcal{U} - 1$, i.e., the deviation from unity of the fraction of reflected power, as a function of the transverse correlation length, a, and the rms height, δ, of the rough surface. The contours are defined by $-10^{-2} < \Delta\mathcal{U} < -10^{-4}$, $-10^{-4} < \Delta\mathcal{U} < 10^{-4}$, $10^{-4} < \Delta\mathcal{U} < 10^{-2}$, and $10^{-2} < \Delta\mathcal{U}$. The results of Fig. 2 were obtained from calculations on a grid of points in parameter space defined by $\delta \in [0.02\lambda, 0.18\lambda]$ and $a \in [0.1\lambda, 2.0\lambda]$ with spacing $\Delta\delta = 0.01\lambda$ and $\Delta a = 0.1\lambda$. For each pair of surface parameters (a, δ), we calculated the fraction of reflected power, $\mathcal{U}$, and averaged the solution over 20 surface realizations. This was found to be sufficient to get convergent results, at least for the surface type and parameters considered in this work.

In the wave scattering from a perfectly conducting substrate, one should formally always have $\mathcal{U} \equiv 1$ independent of the level of surface roughness. However, in numerical calculations this condition may, or may not, be satisfied. The latter case may indicate that the numerical method is being applied outside its range of validity, and that the results cannot be trusted. From Fig. 2 we find that for weakly rough surfaces $\mathcal{U}$ deviates from 1 by less than 10^{-4}, and that the boundary between the regions defined by $|\Delta\mathcal{U}| < 10^{-4}$ and $|\Delta\mathcal{U}| > 10^{-4}$ is approximately given by $\delta = 0.2a$ (indicated by the diagonal dashed line in Fig. 2) for sufficiently small δ/λ.

For a Gaussian correlation function, which was used to produce the results of Fig. 2, the rms slope of the surface is given by $\sqrt{2}\delta/a$ [17]. Thus, the limit of the validity of the Rayleigh hypothesis being given by a linear relationship between δ and a is consistent with the local slope of the surface being the critical parameter. Since the Rayleigh hypothesis is a *small slope* approximation, our finding is not unexpected [4]. For perfectly conducting substrates, we find the Rayleigh hypothesis to be valid for surfaces of rms slope less than about 0.28.

The Rayleigh hypothesis is not expected to introduce any additional restrictions, for example on the amplitude of the rough surface. However, from Fig. 2 we observe that regardless of the correlation length, $\mathcal{U}$ deviates from 1 when $\delta \gtrsim 0.13$. Since this is not an expected consequence of the Rayleigh hypothesis, one may wonder about the cause of this behaviour.

As was discussed in Sec. 3.3, with increasing amplitudes of $\zeta\left(\boldsymbol{x}_{\parallel}\right)$ we no longer expect to be able to accurately calculate the integrals $I(\gamma|\boldsymbol{Q}_{\parallel})$. Preliminary tests indicate that this problem can be alleviated somewhat by increasing the order up to which the sum in (11a) is carried out, but at some point limited numerical precision, leading to numerical cancellations, becomes an issue. Hence, we concluded that the upper finite roughness level for which $\mathcal{U}$ starts deviating significantly from 1 is not a consequence of the Rayleigh hypothesis. Rather, it is a numerical artifact of how the integrals encoding the surface roughness are calculated. We speculate that using an alternative way of calculating $I(\gamma|\boldsymbol{Q}_{\parallel})$ which is not based on a series expansion may resolve this issue, but at the cost of significantly increased computational time. A more promising approach might be to employ software libraries which allow calculations to be carried out with arbitrary precision. Tests we have performed, as well as the results of Ref. 11, indicate that higher precision allows the accurate calculation of the integrals $I(\gamma|\boldsymbol{Q}_{\parallel})$, though again this comes with a price in terms of computational time.

The second set of results that will be presented are for silver substrates. Here the wavelength of the incident light was assumed to be 457.9 nm, for which the dielectric function of silver is $\epsilon_2 = -7.5 + 0.24\mathrm{i}$. In Fig. 3, we present the dependence over parameter space of $\mathcal{U}$, i.e., the fraction of the incident power reflected from randomly rough silver surfaces. Since the silver substrate is absorbing, $\mathcal{U}$ will now in general be less than 1, whereas $\mathcal{U} > 1$ still represents an unphysical situation. Again, the values of the rms height, δ, and transverse correlation length, a, were varied, ranging from 0.02 to 0.18λ in 0.01λ increments for δ, and from 0.1λ to 2.9λ in 0.1λ increments for a. For each pair of values, (a, δ), we calculated $\mathcal{U}$, and averaged the solution over 10 surface realizations. The white area in the upper left corner of Fig. 3 represents values where $\mathcal{U} > 1.1$. The large white area in the bottom right corner of Fig. 3 represents surface parameters for which we did not perform any calculations. This was done to reduce computational time, since we are rather confident that for these parameters we will find $\mathcal{U} < 1$.

For a silver substrate, the region of validity of the Rayleigh hypothesis is less pronounced than for the same geometry but with a perfectly conduction substrate. Unlike in a perfect conductor, light can penetrate into the silver and so-called surface modes can be excited. Changing roughness allows light to couple more or less strongly into intermediate surface modes before being scattered back into the vacuum, and the coupling to surface modes is not only dependent on the amplitude of the surface, but also on the length scale of the surface structures.

Still, with these physical differences between a perfectly conducting and a silver substrate, we observe by comparing Figs. 2 and 3 that the structure of the region of validity of the Rayleigh

hypothesis appears roughly similar. For a silver substrate, it follows from an inspection of Fig. 3 that the region of validity is defined by the intersection between the following two regions: (*i*) $\delta \lesssim 0.08a$ corresponding to a critical rms slope of 0.11; and (*ii*) $\delta \lesssim 0.13\lambda$. Note that the critical rms slope is less for a silver (0.11) than a PEC substrate (0.28), while the second region is the same for the same two substrates.

5. Conclusions

We have presented preliminary results for the numerical investigation of the validity of the Rayleigh hypothesis obtained by studying the fraction of the incident power which is reflected from rough surfaces. In this way it is found that the Rayleigh hypothesis is valid for perfectly conducting substrates when $\delta \lesssim 0.2a$ and for silver substrates when $\delta \lesssim 0.08a$, where δ denotes the rms height and a the correlation length of the surfaces roughness. These regions correspond to critical rms slopes of 0.28 (PEC) and 0.11 (silver), respectively. Both regions are bounded upwards by an rms height of approximately $\delta \approx 0.13\lambda$. We argue that this is not an inherent limitation of the Rayleigh hypothesis, which is a *small-slope* approximation, not a *small-amplitude* approximation, but rather a consequence of the way we calculate the integrals $I(\gamma|\boldsymbol{Q}_{\|})$ [see (11)] present in the reduced Rayleigh equation. It may be possible to get around this limitation by using increased numerical precision, or another algorithm for calculating $I(\gamma|\boldsymbol{Q}_{\|})$, but at the cost of increased computational time.

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