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Considerations to Rayleigh's hypothesis

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ABSTRACT

In 1907 Lord Rayleigh published a paper on the dynamic theory of gratings. In this paper he presented a rigorous approach for solving plane wave scattering on periodic surfaces. Moreover he derived explicit expressions for a perfectly conducting sinusoidal surface, and for perpendicular incidence of the electromagnetic plane wave. This paper was criticized by Lippmann in 1953 for he assumed Rayleigh's approach to be incomplete. Since this time there have been published several arguments, proofs, and discussions concerning the correctness and the range of validity of Rayleigh's approach not only for plane wave scattering on gratings but also for light scattering on nonspherical structures, in general. In the paper at hand we will discuss the different point of views on what is called "Rayleigh's hypothesis" as well as the relevance of a found theoretical limit for its validity. Furthermore we present a numerical treatment of the original scattering problem of a p-polarized plane wave perpendicularly incident on a perfectly conducting sinusoidal surface (i.e., the scalar Dirichlet problem). In doing so we emphasizes the near-field solution especially within the grooves of the grating up to points on the surface, and below the surface. Two different Green's function formulations of Huygens' principle are used as starting points. One of this formulation results in the general T-matrix approach which is considered to be affected by Rayleigh's hypothesis especially for near-field calculations. The other formulation provides a conventional boundary integral equation which is in accordance with Lippmann's point of view and free of problems with Rayleigh's hypothesis. But the obtained results show that Lippmann's argumentation do not withstand a critical numerical analysis, and that the independence of least-squares approaches from Rayleigh's hypothesis, as understood and proven by Millar, seems to hold also for certain methods which does not fit into such an approach.

1. Introduction

This year we celebrate the 100th anniversary of Mie's famous paper in which he solved the light scattering problem on spherical particles rigorously [1]. This paper has become very popular since electromagnetic wave scattering measurements gained more and more importance over the years. To solve the scattering problem Mie applied the well-known separation of variables method in spherical coordinates. Since considering only spherical scatterer he was on the firm mathematical ground of Fourier series to approximate the solution of this specific boundary value problem. But, interestingly, one year before Mie Lord Rayleigh published a paper in which he provided an approach to solve the problem of electromagnetic plane wave scattering from periodic surfaces (gratings) in Cartesian coordinates [2]. Mathematically seen, this is the more complicate boundary value problem since the surface of the grating does not coincide with a constant coordinate line. It is assumed that in this case the separation of variables method cannot be applied successfully. Regardless of such doubts Rayleigh used a series expansion of the scattered wave in terms of outgoing plane waves only, i.e., in terms of waves which move only away from the grating. He determined the unknown expansion coefficients afterwards by application of the boundary conditions at the periodic surface appropriately. For the special case of a perpendicularly incident plane wave on a sinusoidal but perfectly conducting surface he derived an equation system which is at first independent of the groove depth. But Rayleigh approximated this system afterwards to allow for an iterative solution for shallow grooves.

There were no essential arguments against Rayleigh's approach until 1953, when Lippmann published a short note [3] in which he intuitively criticized the usage of solely outgoing plane waves in the representation of the scattered field in the grooves (in space point $\mathbf{r}_1$ in Fig. 1, for example).

Lippmann argued that in the grooves one has to consider also waves which moves toward the surface resulting from surface current elements above the points of observation. Therefore he assumed that Rayleigh's approach is incomplete. This paper can be considered as the hour of birth of the so-called "Rayleigh hypothesis" or "Rayleigh assumption", as the problem was called

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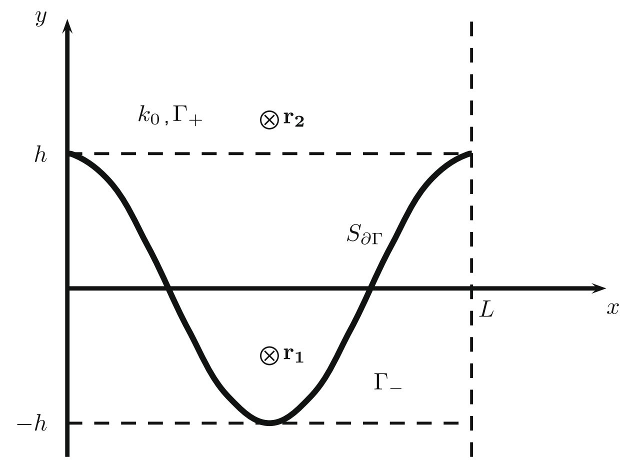

Fig. 1. Geometry of a sinusoidal grating. The boundary surface $S_{\partial\Gamma}$ is given by $y = R(x) = h\cos px$. In Rayleigh's approach solely outgoing plane waves have been considered for the scattered wave everywhere above the surface, i.e., in Γ_+. According to Lippmann's argumentation this is correct only for points above $y = h$ (point $\mathbf{r_2}$). In $\mathbf{r_1}$ one has to consider also incoming waves.

in the manifold discussions and treatments of subsequent papers. Especially the papers of Petit and Cadilhac [4,5], Burrows [6], and Millar [7,8] constituted the next and most essential milestones in this discussion and are cited very often in this context even in recent publications. Petit and Cadilhac presented a mathematical proof of the untenability of Rayleigh's assumption if the product of the amplitude h and the inverse of period L of the grating exceeds a certain value ($h \cdot p > 0.448$; $p = 2\pi/L$). A generalization to the dielectric case can be found in [9]. But there was a numerical development in parallel with seemingly contradictory results. Using Rayleigh's original approach there have been developed certain numerical methods which were able to produce reliable scattering results even if $h \cdot p$ exceeds the theoretical limit of 0.448 [5]. Moreover, Burrows stated in his paper that Rayleigh's approach can be considered to be applicable without any restriction in a generalized sense. But the most detailed treatment was given in the above cited papers by Millar. There we can find a proof of the correctness of Rayleigh's approach if $h \cdot p < 0.448$. This proof was later on simplified and applied to other periodic surfaces as well as to two-dimensional problems by van den Berg and Fokkema [10,11], DeSanto [12], and Keller [13]. The found limit for the validity of Rayleigh's hypothesis is used very often in the literature to justify the restriction of numerical methods but especially that of conventional point-matching. Beside this proof Millar's papers contain additional proofs of the completeness of the outgoing plane waves on the surface of the grating, and of the general possibility to apply a least-squares approach to the boundary condition. This least-squares approach results in a uniformly convergent series expansion of the scattered field in terms of only outgoing plane waves everywhere outside the grating and independent of whether Rayleigh's assumption is fulfilled or not. Especially this last aspect provides an explanation of the above mentioned contradictory results obtained with those numerical methods which fit into a least-squares approach. But in other papers (in [14] chapter 10, for example) we find the statement that convergent results beyond the theoretical groove depth limit can be obtained only for the far-field quantities. This seems to contradict the least-squares proof of Millar. And what happens with the methods which does not fit into a least-squares approach? Some of those methods, including geometric optics approaches, are also able to produce reliable and stable results beyond the theoretical groove depth limit [5,15,16]. Surprisingly, as we will show here, this happens for Rayleigh's original approach for which the limit was claimed to hold. Thus the two questions arise: what does "Rayleigh's hypothesis" really means, and what Rayleigh really did? We are not able here to cite and discuss all the published literature dealing with Rayleigh's hypothesis and its influence on the usefulness or worthlessness of a certain numerical methodology for solving scattering problems on structures which are not appropriate for the separation of variables method. But if one winnows the literature one gets the feeling "that the problem has perhaps been papered over rather than resolved", as Wiscombe and Mugnai stated in [17] when discussing the influence of Rayleigh's hypothesis on Waterman's T-matrix approach [18,19]. T-matrix approaches are of our special interest here since they have become very popular and powerful tools in many applications not at least due to the improvements performed by Mishchenko [20]. But it is also still an open question if these approaches are influenced by Rayleigh's hypothesis and whether they can be used for near-field calculations or not. Such near-field calculations become important if one is interested in plane wave scattering on clusters of particles, for example [20]. It would be of some benefit if those calculations can be performed by use of T-matrix methods.

This somehow muddled situation forced us to treat Rayleigh's original problem (the scalar Dirichlet problem for a p-polarized, perpendicularly incident plane wave) in the chapter after next by three different numerical approaches even in the grooves up to the boundary surface, and beyond. The first one is simply the numerical realization of Rayleigh's original approach. This demonstrates that he used not a least-squares approach but a set of smooth weighting functions in order to fulfil the boundary condition somehow in between a least-squares approach and pointwise. The second approach we use to solve the problem is a least-squares approach. It differs from Rayleigh's approach only in the choice of the weighting functions. Thus we can demonstrate that the choice of the weighting functions has a major impact on the stability and reliability of the results – a fact which is well-known to practitioners, of course. Finally we solve the problem by a boundary integral equation method which is considered to be generally not influenced by Rayleigh's hypothesis, and, therefore, in agreement with Lippmann's requirement to take not only outgoing but also incoming plane waves into account. But there are no differences even in the grooves between all three approaches, as we will see. This gives us the justification to take up a pragmatic position regarding the problem of "Rayleigh's hypothesis".

2. The Rayleigh hypothesis

After two equivalent formulations of the scattering problem of a p-polarized plane wave perpendicularly incident on a sinusoidal and perfectly conducting surface we will derive the general T-matrix approach by use of a rigorous Green's function formalism. Afterwards we discuss the different understandings of the term "Rayleigh hypothesis" in the papers by Lippmann and Millar cited already in Section 1.

2.1. Conventional formulation of the scattering problem

The scattering configuration is depicted in Fig. 2. The scattering problem of a p-polarized plane wave perpendicularly incident from above on a sinusoidal and perfectly conducting surface can be related to the following Dirichlet problem of the homogeneous Helmholtz equation: We are seeking for a solution $u(\mathbf{r})$ in Γ_+ of

$$\nabla^2 u(\mathbf{r}) + k_0^2 u(\mathbf{r}) = 0 \tag{1}$$

with

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}, \tag{2}$$

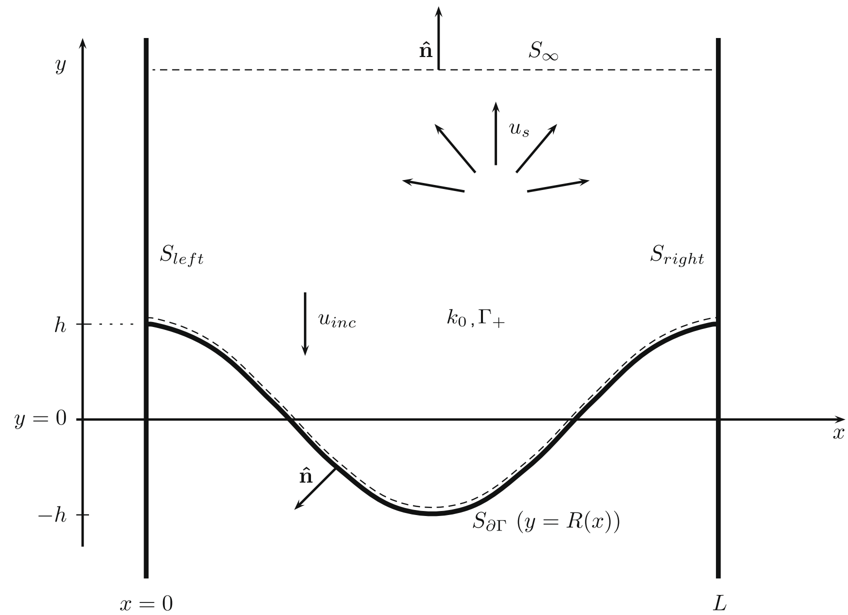

Fig. 2. Scattering configuration of a sinusoidal surface.

and $\mathbf{r}$ being the two-dimensional vector (x, y). The assumed time dependence $exp(-i\omega t)$ is suppressed throughout the paper. The open region Γ_+ above the periodic surface $S_{\partial\Gamma}$ is characterized by the free-space wave number $k_0 = 2\pi/\lambda$. On the periodic boundary we have to fulfil the homogeneous Dirichlet condition

$$u(x, R(x)) = 0. \tag{3}$$

Due to the linearity of Maxwell's equations we can represent the solution $u(\mathbf{r})$ as a superposition of the incident and scattered field,

$$u(\mathbf{r}) = u_{inc}(\mathbf{r}) + u_s(\mathbf{r}). \tag{4}$$

$$u_{inc}(\mathbf{r}) = e^{-ik_0 y} \tag{5}$$

is the given plane wave perpendicularly incident from above the periodic surface. This plane wave is obviously a solution of the homogeneous Helmholtz equation. Furthermore, due to the periodicity of the problem we require

$$u(0, y) = u(L, y) \tag{6}$$

with respect to x. Thus we can approximate $u(\mathbf{r})$ by

$$u(\mathbf{r}) = u_{inc}(\mathbf{r}) + \sum_{n=-N}^{N} u_n(y) \cdot e^{ik_{xn}x} \tag{7}$$

with

$$k_{xn} = np; \quad p = \frac{2\pi}{L}, \tag{8}$$

and N being a finite number. The appropriate choice of N is discussed in the next chapter when dealing with the numerical realization of certain methods. We need an additional condition in order to specify $u_n(y)$ in the series expansion of the scattered field. This is the non-local radiation condition

$$\lim_{y\to\infty}\left(\frac{\partial u_n(y)}{\partial y} - ik_{yn}u_n(y)\right) = 0. \tag{9}$$

S_∞ is considered to be this outer but non-local boundary of Γ_+. The discrete values of k_{yn} are defined according to

$$k_{yn} = \begin{cases} \sqrt{k_0^2 - k_{xn}^2}; & \text{if } k_0^2 > k_{xn}^2 \\ i\sqrt{k_{xn}^2 - k_0^2}; & \text{if } k_{xn}^2 > k_0^2. \end{cases} \tag{10}$$

This condition is fulfilled by every outgoing plane wave

$$u_n(y) = a_n \cdot e^{ik_{yn}y} \tag{11}$$

with constant a_n. But it is not fulfilled by the total field $u(\mathbf{r})$ since the incident plane wave (5) violates this condition. Inserting (11) into the series expansion of the scattered field in Eq. (7) provides the representation

$$u_s(x, y) = \sum_{n=-N}^{N} a_n^{(N)} \cdot e^{i(k_{xn}x + k_{yn}y)} \tag{12}$$

which is assumed to applies generally for every $y > h$. Since the boundary surface $S_{\partial\Gamma}$ of our interest is given by the even function

$$y = R(x) = h\cos px, \tag{13}$$

and since considering perpendicular incidence of the plane wave $a_n^{(N)} = a_{-n}^{(N)}$ holds, i.e., the scattered modes are symmetric with respect to the y-axis. Thus we can rewrite representation (12) as follows:

$$\begin{aligned} u_s(x, y) &= \sum_{n=0}^{N} a_n^{(N)} \cdot e^{i(k_{xn}x + k_{yn}y)} + \sum_{n=1}^{N} a_n^{(N)} \cdot e^{i(-k_{xn}x + k_{yn}y)} \\ &= \sum_{n=0}^{N} a_n^{(N)} \cdot \epsilon_n \cdot \cos k_{xn}x \cdot e^{ik_{yn}y}. \end{aligned} \tag{14}$$

Here we have $\epsilon_n = 1$ if $n = 0$, and $\epsilon_n = 2$ if $n > 0$. This last representation was used by Rayleigh in [2]. Before discussing different methods to calculate the unknown coefficients $a_n^{(N)}$ we will formulate the problem again by applying Green functions.

2.2. Formulation of the scattering problem in terms of Green functions

In contrast to (1) we ask now for the solution of the inhomogeneous Helmholtz equation

$$\nabla^2 u(\mathbf{r}) + k_0^2 u(\mathbf{r}) = -\rho(\mathbf{r}) \tag{15}$$

subject to the Dirichlet condition (3), the periodicity condition (6), and the radiation condition (9). $\rho(\mathbf{r})$ is the source which generates the primary incident field u_{inc}, i.e., u_{inc} is a solution of

$$\nabla^2 u_{inc}(\mathbf{r}) + k_0^2 u_{inc}(\mathbf{r}) = -\rho(\mathbf{r}) \tag{16}$$

The necessity of introducing a local source is a consequence of the cause and action concept of Green's functions. We will now express the incident field u_{inc} as well as the total field u by use of appropriate Green functions.

2.2.1. Free-space Green's function and the incident plane wave

It should be emphasized that for the scattering problem under consideration the free-space Green's function depends on the direction of incidence of the plane wave. This is a consequence of the restriction to a space with only periodic functions (fields and sources). All ongoing discussions and representations of G_0 are therefore restricted to perpendicular incidence only!

Let us see now how we can generate the plane wave (5) perpendicularly incident on the periodic boundary (13). For this we introduce the free-space Green's function by the defining equation

$$\nabla^2_{\mathbf{r}} G_0(\mathbf{r},\mathbf{r}') + k_0^2 G_0(\mathbf{r},\mathbf{r}') = -\delta(\mathbf{r}-\mathbf{r}'). \tag{17}$$

This Green's function is related to the whole space $\Gamma = \Gamma_+ \cup \Gamma_-$ without the grating (i.e., the unperturbed problem). But despite of this we require the fulfilment of the periodicity condition

$$G_0(0,y;\mathbf{r}') = G_0(L,y;\mathbf{r}') \tag{18}$$

with respect to x. Due to this condition we can expand G_0 into the Fourier series

$$G_0(\mathbf{r},\mathbf{r}') = \sum_{n=-\infty}^{\infty} G_n(y,\mathbf{r}') \cdot e^{ik_{xn}x}. \tag{19}$$

The $G_n(y,\mathbf{r}')$ have to fulfil the radiation condition

$$\lim_{|y|\to\infty}\left(\frac{\partial G_n(y,\mathbf{r}')}{\partial |y|} - ik_{yn}G_n(y,\mathbf{r}')\right) = 0 \tag{20}$$

which holds at S_∞ as well as at $S_{-\infty}$ [21]. In the literature one can find several expressions for this Green's function (for an overview, see [22]). Here we want to employ the expression

$$G_0(\mathbf{r},\mathbf{r}') = \frac{i}{2L}\cdot\sum_{n=0}^{\infty}\frac{\epsilon_n}{k_{yn}}\cos k_{xn}(x-x')e^{ik_{yn}|y-y'|}. \tag{21}$$

Please, note that the $e^{ik_{xn}x}$ term in (19) has been resolved into the term $\cos k_{xn}(x-x')$ thus restricting the sum over n to run from 0 to ∞. The values of ϵ_n are defined as in Eq. (14). This representation of G_0 does not explicitely show the expected logarithmic singularity at $\mathbf{r}=\mathbf{r}'$. But it is obviously divergent in this point. Moreover, it exhibits the symmetry

$$G_0(\mathbf{r},\mathbf{r}') = G_0(\mathbf{r}',\mathbf{r}) \tag{22}$$

which follows from application of Green's theorem

$$\int_\Gamma \left[\Psi(\mathbf{r})\nabla^2\Phi(\mathbf{r}) - \Phi(\mathbf{r})\nabla^2\Psi(\mathbf{r})\right]dV(\mathbf{r}) = \oint_S \left[\Psi(\mathbf{r})\frac{\partial\Phi(\mathbf{r})}{\partial\hat{\mathbf{n}}} - \Phi(\mathbf{r})\frac{\partial\Psi(\mathbf{r})}{\partial\hat{\mathbf{n}}}\right]dS(\mathbf{r}). \tag{23}$$

in $\Gamma = \Gamma_+ \cup \Gamma_-$ with

$$\Psi(\mathbf{r}) = G_0(\mathbf{r},\mathbf{r}') \tag{24}$$

$$\Phi(\mathbf{r}) = G_0(\mathbf{r},\mathbf{r}''), \tag{25}$$

and in conjunction with the radiation condition (20) and periodicity condition (18). The closed boundary S of the surface integral on the right-hand side of (23) consists of the parts S_{right}, S_{left}, S_∞, and $S_{-\infty}$ (see Fig. 3). The derivation with respect to the unit normal vector is defined according to

$$\frac{\partial\Phi}{\partial\hat{\mathbf{n}}} := \hat{\mathbf{n}}\cdot\nabla\Phi. \tag{26}$$

On the other hand, if we choose

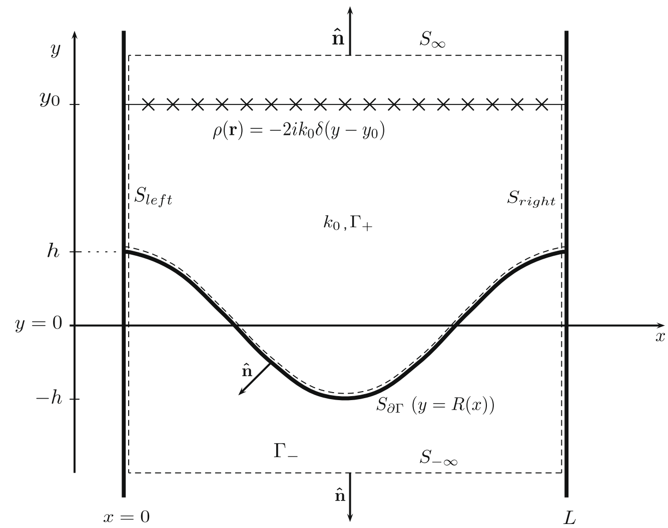

Fig. 3. Scattering configuration of a sinusoidal surface if formulated in terms of Green functions.

$$\Psi(\mathbf{r}) = G_0(\mathbf{r},\mathbf{r}') \tag{27}$$

$$\Phi(\mathbf{r}) = u_{inc}(\mathbf{r}) \tag{28}$$

in (23), we get

$$u_{inc}(\mathbf{r}) = \int_\Gamma G_0(\mathbf{r},\mathbf{r}')\cdot\rho(\mathbf{r}')dV(\mathbf{r}') \tag{29}$$

If taking the symmetry (22) and Eqs. (16) and (17) into account, and if requiring the radiation condition (20) to hold also for u_{inc}. Then it is straightforward to show that the source distribution

$$\rho(\mathbf{r}) = -2ik_0\delta(y-y_0) = -2ik_0\cdot\cos k_{x0}x\cdot\delta(y-y_0) \tag{30}$$

in conjunction with expression (21) generates the incident field

$$u_{inc}(\mathbf{r}) = e^{ik_0|y-y_0|}. \tag{31}$$

If we locate y_0 somewhere in Γ_+ such that

$$y_0 > h, \tag{32}$$

and if choosing w.l.o.g.

$$e^{ik_0y_0} = 1 \tag{33}$$

(see Fig. 3) we produce exactly the incident field (5) below y_0 needed for our discussion.

But representation (21) can be simplified further. Due to the considered surface (13) it is sufficient to take only the even part

$$\widetilde{G}_0(\mathbf{r},\mathbf{r}') = \frac{i}{2L}\cdot\sum_{n=0}^{\infty}\frac{\epsilon_n}{k_{yn}}\cos k_{xn}x\cos k_{xn}x'e^{ik_{yn}|y-y'|} \tag{34}$$

of G_0 with respect to x into account. This expression can be decomposed into

$$\widetilde{G}_0(\mathbf{r},\mathbf{r}') = \begin{cases}\widetilde{G}_0^>(\mathbf{r},\mathbf{r}'); & y > y'\\ \widetilde{G}_0^<(\mathbf{r},\mathbf{r}'); & y < y',\end{cases} \tag{35}$$

with

$$\widetilde{G}_0^>(\mathbf{r},\mathbf{r}') = \frac{i}{2L}\cdot\sum_{n=0}^{\infty}\tilde{\phi}_n(\mathbf{r})\cdot\tilde{\psi}_n(\mathbf{r}') \tag{36}$$

$$\widetilde{G}_0^<(\mathbf{r},\mathbf{r}') = \frac{i}{2L}\cdot\sum_{n=0}^{\infty}\tilde{\psi}_n(\mathbf{r})\cdot\tilde{\phi}_n(\mathbf{r}'). \tag{37}$$

The expansion functions therein are given by

$$\tilde{\phi}_n(\mathbf{r}) = \sqrt{\frac{\epsilon_n}{k_{yn}}} \cdot \phi_n(\mathbf{r}) \tag{38}$$

$$\phi_n(\mathbf{r}) = \cos k_{xn}x e^{ik_{yn}y} \tag{39}$$

$$\tilde{\psi}_n(\mathbf{r}) = \sqrt{\frac{\epsilon_n}{k_{yn}}} \cdot \psi_n(\mathbf{r}) \tag{40}$$

$$\psi_n(\mathbf{r}) = \cos k_{xn}x e^{-ik_{yn}y}. \tag{41}$$

This even part of G_0 together with the source distribution (30) produces the same incident field (5) below y_0.

2.2.2. Green's function of the total field in Γ_+

The Green's function which is related to the considered scattering problem in Γ_+ is also a solution of the inhomogeneous Helmholtz equation

$$\nabla^2_{\mathbf{r}} G_+(\mathbf{r},\mathbf{r}') + k_0^2 G_+(\mathbf{r},\mathbf{r}') = -\delta(\mathbf{r}-\mathbf{r}'). \tag{42}$$

Γ_+ is enclosed by S_{right}, S_{left}, S_∞, and $S_{\partial\Gamma}$. We require again the fulfilment of the periodicity condition

$$G_+(0,y;\mathbf{r}') = G_+(L,y;\mathbf{r}') \tag{43}$$

with respect to x as well as the radiation condition (9) if $y \to \infty$. But in contrast to the free-space Green's function we have the additional homogeneous Dirichlet condition

$$G_+(x,R(x);\mathbf{r}') = 0 \tag{44}$$

which must hold on the surface of the grating. G_+ obeys the symmetry relation we already know from G_0, i.e.,

$$G_+(\mathbf{r},\mathbf{r}') = G_+(\mathbf{r}',\mathbf{r}). \tag{45}$$

This can be simply proven by using

$$\Psi(\mathbf{r}) = G_+(\mathbf{r},\mathbf{r}') \tag{46}$$

$$\Phi(\mathbf{r}) = G_+(\mathbf{r},\mathbf{r}''), \tag{47}$$

in Green theorem (23) now applied in Γ_+. On the other hand, if using

$$\Psi(\mathbf{r}) = G_+(\mathbf{r},\mathbf{r}') \tag{48}$$

$$\Phi(\mathbf{r}) = u(\mathbf{r}) \tag{49}$$

in (23), we get

$$u(\mathbf{r}) = \int_{\Gamma_+} G_+(\mathbf{r},\mathbf{r}') \cdot \rho(\mathbf{r}') dV(\mathbf{r}'). \tag{50}$$

The problem we have to solve now is the determination of the unknown Green's function G_+. For this we introduce the so-called interaction operator $W_{\partial\Gamma}$ by the definition (see [23], for example)

$$G_+(\mathbf{r},\mathbf{r}') := \widetilde{G}_0(\mathbf{r},\mathbf{r}') + \int_{S_{\partial\Gamma}} \widetilde{G}_0(\mathbf{r},\hat{\mathbf{r}}) \cdot W_{\partial\Gamma}(\hat{\mathbf{r}},\tilde{\mathbf{r}}) \cdot \widetilde{G}_0(\tilde{\mathbf{r}},\mathbf{r}') dS(\hat{\mathbf{r}}) dS(\tilde{\mathbf{r}}). \tag{51}$$

This interaction operator is solely determined on the surface of the grating and describes the interaction of the incident plane wave with this surface. For $\mathbf{r}$ not on the surface and $\mathbf{r}'$ being the location of the primary source (30) this representation of G_+ is in accordance with all requirements formulated above. For the ongoing discussion we assume generally that $y < y_0$ holds. Thus we can write instead of (51)

$$G_+(\mathbf{r},\mathbf{r}') = \widetilde{G}_0^<(\mathbf{r},\mathbf{r}') + \int_{S_{\partial\Gamma}} \widetilde{G}_0(\mathbf{r},\hat{\mathbf{r}}) \cdot W_{\partial\Gamma}(\hat{\mathbf{r}},\tilde{\mathbf{r}}) \cdot \widetilde{G}_0^<(\tilde{\mathbf{r}},\mathbf{r}') dS(\hat{\mathbf{r}}) dS(\tilde{\mathbf{r}}). \tag{52}$$

Please, note that on the surface $R(x)$ of the grating we have the unit normal vector

$$\hat{\mathbf{n}} = \frac{\hat{\mathbf{e}}_x \cdot R'(x) - \hat{\mathbf{e}}_y}{\sqrt{1+[R'(x)]^2}} \tag{53}$$

with $R\prime(x) = dR(x)/dx$. The surface element dS in the surface integral on the right-hand side of (51)/(52) is given by

$$dS(\mathbf{r}) = \sqrt{1+[R\prime(x)]^2}dx = S(x)dx. \tag{54}$$

If we further restrict the variable y to the region in Γ_+ for which $y > h$ holds we can replace $\widetilde{G}_0(\mathbf{r},\hat{\mathbf{r}})$ in the surface integral of (52) by $\widetilde{G}_0^>(\mathbf{r},\hat{\mathbf{r}})$, i.e.,

$$G_+(\mathbf{r},\mathbf{r}') = \widetilde{G}_0^<(\mathbf{r},\mathbf{r}') + \int_{S_{\partial\Gamma}} \widetilde{G}_0^>(\mathbf{r},\hat{\mathbf{r}}) \cdot W_{\partial\Gamma}(\hat{\mathbf{r}},\tilde{\mathbf{r}}) \cdot \widetilde{G}_0^<(\tilde{\mathbf{r}},\mathbf{r}') dS(\hat{\mathbf{r}}) dS(\tilde{\mathbf{r}}). \tag{55}$$

If using expansions (36) and (37) but now truncated at a finite number N, and if defining the matrix elements of the interaction operator according to

$$[W_{\partial\Gamma}]_{n,n'} := \frac{i}{2L} \int_{S_{\partial\Gamma}} \tilde{\psi}_n(\hat{x},R(\hat{x})) \cdot W_{\partial\Gamma}(\hat{\mathbf{r}},\tilde{\mathbf{r}}) \cdot \widetilde{\psi}_{n'}(\tilde{x},R(\tilde{x})) dS(\hat{\mathbf{r}}) dS(\tilde{\mathbf{r}}) \tag{56}$$

we get as an approximation of G_+ in the considered region $y > h$

$$G_+^{(N)}(\mathbf{r},\mathbf{r}') = \widetilde{G}_0^<(\mathbf{r},\mathbf{r}') + \frac{i}{2L} \cdot \sum_{n,n'=0}^{N} [W_{\partial\Gamma}]_{n,n'} \cdot \widetilde{\phi}_n(\mathbf{r}) \cdot \widetilde{\phi}_{n'}(\mathbf{r}'). \tag{57}$$

This is a representation in terms of outgoing plane waves only with respect to y and y'. Inserting this expression together with the source distribution (30) into (50) provides the corresponding representation

$$u(\mathbf{r}) = u_{inc} + \sqrt{k_0} \cdot \sum_{n=0}^{N} \sqrt{\frac{\epsilon_n}{k_{yn}}} \cdot [W_{\partial\Gamma}]_{n,0} \cdot \phi_n(\mathbf{r}) \tag{58}$$

of the total field in the region $h < y < y_0$. The second part on the right-hand side of this equation represents the scattered field. If comparing it with (14) we get

$$a_n^{(N)} = \sqrt{\frac{k_0}{k_{yn}\epsilon_n}} \cdot [W_{\partial\Gamma}]_{n,0} \tag{59}$$

as the relation between the expansion coefficients in Rayleigh's representation and the matrix elements of the interaction operator. Thus we can state that in region $h < y < y_0$ representation (55) or approximation (57) of the Green's function related to our scattering problem is equivalent to the conventional representation of the total field with the scattered part given by (14). But the question how to determine the unknown expansion coefficients or the matrix elements (56) of the interaction operator, respectively, is still open. This will be considered now.

2.3. T-matrices and Rayleigh's method

In this subchapter we will first discuss the general T-matrix approach. It turns out afterwards that Rayleigh's original approach is nothing but a certain realization of this method. To demonstrate this we have to choose the weighting functions appropriately. Two other choices of weighting functions are also discussed which result in other T-matrices.

The essential step to determine the unknown coefficients is the following assumption which dates back to Rayleigh:

- **Representation (14) holds not only for $y > h$ but also for all values of y within the grooves and at the surface of the grating.**

To determine the matrix elements of the interaction operator we formulate the equivalent assumption for the Green's function of the scattering problem:

- **Representation**

$$G_+^R(\mathbf{r},\mathbf{r}') = \widetilde{G}_0^<(\mathbf{r},\mathbf{r}') + \int_{S_{\partial\Gamma}} \widetilde{G}_0^>(\mathbf{r},\hat{\mathbf{r}}) \cdot W_{\partial\Gamma}^R(\hat{\mathbf{r}},\tilde{\mathbf{r}}) \cdot \widetilde{G}_0^<(\tilde{\mathbf{r}},\mathbf{r}') dS(\hat{\mathbf{r}}) dS(\tilde{\mathbf{r}}), \tag{60}$$

or, equivalently, approximation (57) holds not only for $y > h$ but also for all values of y within the grooves and at the surface of the grating.

Please, note that the Green's function as well as the matrix elements (56) of the interaction operator are marked with the upper letter "R" to distinguish the resulting approach from the approach on the basis of Lippmann's argumentation we will consider later on. We will call both assumptions "Rayleigh's assumption". They allow us to apply the additional Dirichlet conditions (3) or (44), respectively, to determine the unknown quantities. The matrix elements of the interaction operator can thus be determined in the following way:

Applying (44) to (57) provides the equation

$$\sum_{n'=0}^{N} \tilde{\psi}_{n'}(x,R(x)) \cdot \tilde{\phi}_{n'}(\mathbf{r}') = -\sum_{n,n'=0}^{N} \tilde{\phi}_n(x,R(x)) \cdot [W_{\partial\Gamma}^R]_{n,n'} \cdot \tilde{\phi}_{n'}(\mathbf{r}') \tag{61}$$

if using the (now finite!) expansion (37) to approximate $\widetilde{G}_0^<(\mathbf{r},\mathbf{r}')$ in Eq. (57). Next we ask for the transformation matrix $\widetilde{\mathbf{T}}_{\partial\Gamma}$ which allows us to express the expansion functions $\tilde{\psi}_{n'}(x,R(x))$ by the expansion functions $\tilde{\phi}_n(x,R(x))$ on the surface $y = R(x)$ of the grating according to

$$\tilde{\psi}_{n'}(x,R(x)) \cong \sum_{n=0}^{N} [\widetilde{T}_{\partial\Gamma}]_{n',n} \tilde{\phi}_n(x,R(x)), \tag{62}$$

where the "equal"-sign holds only for a plane interface $R(x) = const$. If we insert this relation into (61) we get after comparison

$$[W_{\partial\Gamma}^R]_{n,n'} = -[T_{\partial\Gamma}]_{n,n'} = -[\widetilde{T}_{\partial\Gamma}]_{n,n'}^{tp}. \tag{63}$$

Index "tp" denotes the transpose of $[\widetilde{T}_{\partial\Gamma}]_{n,n'}$. $[T_{\partial\Gamma}]_{n',n}$, on the other hand, can be calculated according to (see [18,23,24], for example)

$$[T_{\partial\Gamma}]_{n,n'} = \sum_{m=0}^{N} [A_{\partial\Gamma}^{-1}]_{n,m} [B_{\partial\Gamma}]_{m,n'} \tag{64}$$

from the two matrices $\mathbf{A}_{\partial\Gamma}$ and $\mathbf{B}_{\partial\Gamma}$. Their elements are given by

$$[A_{\partial\Gamma}]_{n,m} = \langle w_n(\mathbf{r}) | \tilde{\phi}_m(\mathbf{r}) \rangle \tag{65}$$

$$[B_{\partial\Gamma}]_{n,m} = \langle w_n(\mathbf{r}) | \tilde{\psi}_m(\mathbf{r}) \rangle \tag{66}$$

with the scalar product defined according to

$$\langle w_n(\mathbf{r}) | f_m(\mathbf{r}) \rangle := \frac{1}{L} \cdot \int_0^L w_n^*(x,R(x)) \cdot f_m(x,R(x)) dx. \tag{67}$$

In contrast to the way described above Waterman employed the so-called "Extended Boundary Condition" in his original papers. But the result is still the same, as proven for three-dimensional scattering problems in [25], for example. As it can be seen from (59) it is sufficient to know only the first column of the matrix $\mathbf{W}_{\partial\Gamma}^{\mathbf{R}}$, i.e., we need only

$$[T_{\partial\Gamma}]_{n,0} = \sum_{m=0}^{N} [A_{\partial\Gamma}^{-1}]_{n,m} \cdot [B_{\partial\Gamma}]_{m,0}. \tag{68}$$

Moreover, in (64)/(68) we have the degree of freedom to choose the set of weighting functions $\{w_n(\mathbf{r})\}_{n=0}^N$ appropriately. Due to our special scattering surface they are only restricted to be even functions with respect to x. Three types of weighting functions are of our special interest here:

Let

$$w_n(\mathbf{r}) = L \cdot \delta(x - x_n) \tag{69}$$

with x_n being $N+1$ points within the interval $[0,L)$. These weighting functions provides the conventional point-matching technique, as can be seen from (68) in conjunction with (65), (66), and (38)–(41). This technique was the catalyst of a controversial discussion by Bates and Millar [26] and of Millar's analysis of Rayleigh's hypothesis. It is well-known by practitioners that this method is not very stable and provides accurate results only for shallow gratings. But a drastic improvement can be achieved if the number of points chosen on the surface exceeds the number of unknowns in the series expansion (14) of the scattered field thus getting an overdetermined equation system. Applying to this system a least-squares approach (a singular value decomposition procedure, for example) results in a much more stable method which is called the "improved" or "generalized" point-matching technique. An essential characteristics of both methods is the fact that the resulting expansion coefficients are not final, i.e., that they are dependent on the number N of expansion terms used in the representation of the scattered field. Thus, if the problem requires the consideration of an additional expansion term all coefficients must be calculated again. This is the reason why we denoted the expansion coefficients in (12), (14), and in (59) with $a_n^{(N)}$.

$$w_n(\mathbf{r}) = \cos k_{xn} x \tag{70}$$

is another type of weighting functions of our interest. Taking the integral representation

$$\frac{1}{2\pi} \cdot \int_0^{2\pi} e^{i(ny - z\cos y)} dy = e^{-i(n\pi)/2} \cdot J_n(z) \tag{71}$$

of Bessel's functions $J_n(z)$ into account we get from (65) and (66)

$$[A_{\partial\Gamma}]_{m,n} = \frac{1}{2}\sqrt{\frac{\epsilon_n}{k_{yn}}} \{ e^{i(m+n)\frac{\pi}{2}} \cdot J_{m+n}(hk_{yn}) + e^{i(m-n)\frac{\pi}{2}} \cdot J_{m-n}(hk_{yn}) \} \tag{72}$$

$$[B_{\partial\Gamma}]_{m,n} = \frac{1}{2}\sqrt{\frac{\epsilon_n}{k_{yn}}} \{ e^{-i(m+n)\frac{\pi}{2}} \cdot J_{m+n}(hk_{yn}) + e^{-i(m-n)\frac{\pi}{2}} \cdot J_{m-n}(hk_{yn}) \} \tag{73}$$

as the relevant matrix elements. Albeit of our more compact notation this agrees exactly with the equation system derived by Rayleigh in his original paper (see Eqs. (28)–(34) in [2]). It should be mentioned that Rayleigh applied the Jacobi-Anger formula instead of Sommerfeld's integral representation to derive the equation system. This system was resolved afterwards by Rayleigh under the assumption of a shallow grating. This allowed him to derive explicit expressions for the expansion coefficients according to (59). We have to state again that the resulting expansion coefficients are not final! It should be also mentioned that these weighting functions does not belong to a least-squares scheme.

Therefore, let

$$w_n(\mathbf{r}) = \tilde{\phi}_n(x,R(x)) \tag{74}$$

with $\tilde{\phi}_n$ according to (38). This choice of weighting functions corresponds to the least-squares determination of $\widetilde{\mathbf{T}}_{\partial\Gamma}$ in (62). We are again able to perform the scalar product in (65) and (66) analytically. The matrix elements read in this case

$$[A_{\partial\Gamma}]_{m,n} = \frac{1}{2}\sqrt{\frac{\epsilon_n\epsilon_m}{k_{yn}k_{ym}}} \Big\{ e^{i(m+n)\frac{\pi}{2}} \cdot J_{m+n}(h(k_{yn} - k_{ym}^*)) + e^{i(m-n)\frac{\pi}{2}} \cdot J_{m-n}(h(k_{yn} - k_{ym}^*)) \Big\} \tag{75}$$

$$[B_{\partial\Gamma}]_{m,n} = \frac{1}{2}\sqrt{\frac{\epsilon_n\epsilon_m}{k_{yn}k_{ym}}} \Big\{ e^{-i(m+n)\frac{\pi}{2}} \cdot J_{m+n}(h(k_{yn} + k_{ym}^*)) + e^{-i(m-n)\frac{\pi}{2}} \cdot J_{m-n}(h(k_{yn} + k_{ym}^*)) \Big\} \tag{76}$$

and the corresponding expansion coefficients are again not final. Other types of T-matrices which can be related to other choices of weighting functions are described in [27], for example.

The numerical realization and consequences of these choices of weighting functions will be discussed in chapter 3. But before doing this we are now prepared to discuss the two different understanding of "Rayleigh's hypothesis" in Petit's/Cadilhac's/Millar's, and in Lippmann's initially mentioned papers.

2.4. Rayleigh's hypothesis according to Petit, Cadilhac, and Millar

In [4,5,7,8] the authors started from the representation

$$u_s(x,y) = \sum_{n=-\infty}^{\infty} a_n \cdot e^{i(k_{xn}x - k_{yn}y)}. \tag{77}$$

of the scattered field in terms of outgoing waves only. It differs from our representation (12) by assuming an infinite expansion from the beginning with final expansion coefficients. Moreover, applying Green's theorem (23) in a subdomain of Γ_+ bounded by S_{left}, S_{right}, $S_{\partial\Gamma}$, and $h < y \leqslant const. < y_0$ with

$$\Psi(\mathbf{r}) = u_s(\mathbf{r}), \tag{78}$$
$$\Phi(\mathbf{r}) = e^{-i(k_{xn}x - k_{yn}y)}. \tag{79}$$

Millar could relate the final coefficients to the surface integral

$$a_n = \frac{i}{2k_{yn}L} \cdot \int_{S_{\partial\Gamma}} \left[u_s(\mathbf{r}) \frac{\partial}{\partial \hat{n}} - \frac{\partial u_s(\mathbf{r})}{\partial \hat{n}} \right] \cdot e^{i(k_{xn}x - k_{yn}y)} dS(\mathbf{r}) \tag{80}$$

containing the known scattered field u_s and its unknown outward normal derivative on the surface $S_{\partial\Gamma}$ (see [7,8]). Rayleigh's hypothesis in the understanding of Petit, Cadilhac, and Millar is defined as follows (if we talk about Rayleigh's hypothesis in the ongoing discussion of this subchapter this definition is tacitly meant!):

It is the assumption that expansion (77) with coefficients (80) is a valid representation of u_s not only in $y > h$ but in every point of Γ_+ and especially on the surface $R(x)$ [8]. Thus the Dirchlet condition (3) provides

$$e^{-ik_0R(x)} = -\sum_{n=-\infty}^{\infty} a_n \cdot e^{i(k_{xn}x - k_{yn}R(x))} \tag{81}$$

which is assumed further to hold **in every point** of this surface.

This understanding of Rayleigh's hypothesis targeted obviously at conventional point-matching methods [28]. According to our discussion in the foregoing subchapter this designation is somehow questionable since Rayleigh never used the conventional point-matching method nor he assumed final expansion coefficients according to (80) even if he did not made it in his equations. Some misunderstandings in the recent literature may result from this confusing designation. But for practitioners operating with conventional point-matching methods the analysis of Petit, Cadilhac, and Millar is of importance since Petit and Cadilhac found a counter example, i.e., a point on the surface which violates boundary condition (81). They could show in an elegant way that in $x = L/2$ condition (81) is violated if $h \cdot p > 0.448$ [4,5]. Millar, on the other hand, could show by inspection of the singularities of the scattered field that Rayleigh's hypothesis as formulated above holds for $h \cdot p < 0.448$ [7]. Thus $h \cdot p = 0.448$ can be considered to be an upper limit of the applicability of conventional point-matching techniques even though they never reach this value in practical calculations since running into stability problems much before. Excluding such critical surface points in the corresponding procedure would be therefore of little benefit. This is the reason why conventional point-matching methods are nowadays of less importance. But the requirement that boundary condition (81) must hold in every point on the surface is questionable also from a more physical point of view. Sommerfeld stated in [21] that "*in mathematical lectures on Fourier series emphasis is usually put on the concept of arbitrary functions, on its continuity properties and its singularities. This point of view becomes immaterial in the physical applications. For, the initial boundary values of functions... must always be taken as smoothed mean values, just as the partial differential equations in which they enter arise from a statistical averaging of much more complicated elementary laws. Hence we are concerned with relatively simple idealized functions and with their approximation with... "Method of Least Squares". We shall see that it opens a simple and rigorous approach not only to Fourier series but to all other series expansions of mathematical physics... in eigenfunctions*".

This physical point of view is reflected in Millar's proof that an understanding of boundary condition (81) in a least-squares sense, i.e.,

$$e^{-ik_0R(x)} = -\sum_{n=-N}^{N} a_n^{(N)} \cdot e^{i(k_{xn}x - k_{yn}R(x))} = u_s^{(N)}(R(x)) \tag{82}$$

with coefficients $a_n^{(N)}$ calculated by minimizing the least-squares norm

$$\sqrt{\langle u_{inc}(R(x)) + u_s^{(N)}(R(x)) \mid u_{inc}(R(x)) + u_s^{(N)}(R(x)) \rangle} \tag{83}$$

is generally not influenced by Rayleigh's hypothesis and results in a representation of the scattered field everywhere above $y = R(x)$ which converges uniformly against the exact solution [8]. Please, note that the scalar product $\langle g(\mathbf{x}) \mid f(\mathbf{x}) \rangle$ was already defined in (67). T-matrix methods which are based on the third choice (74) of weighting functions as well as generalized point-matching procedures are therefore not in conflict with Rayleigh's hypothesis. Rayleigh's original approach is somewhere in between conventional point-matching and least-squares methods and provide stable results much beyond the limit of Petit, Cadilhac, and Millar. But as we will demonstrate in our numerical analysis the region of stable and convergent results depends strongly on the choice of weighting functions. And it is known from practical applications that a least-squares approach is not necessarily the best one (see [29], for example).

In this context it should be mentioned that one can find in the more mathematical-oriented literature the following abstract definition of Rayleigh's hypothesis (see [24], for example): If the outgoing plane wave functions form a Schauder basis for $L_2(\partial\Gamma)$ (that is the space of all square-integrable functions on $S_{\partial\Gamma}$) Rayleigh's hypothesis (or, better, Rayleigh's assumption that the expansion of the scattered field in terms of outgoing plane waves only is able to solve the scattering problem) is said to be satisfied. An infinite set of functions f_n form a Schauder basis if there is a unique set of final coefficients a_n such that any function u on the surface of the grating can be represented by

$$u = \sum_{n=0}^{\infty} a_n \cdot f_n \tag{84}$$

(see [30], for example). What does it means from a more practical point of view? We would then be able to apply the T-matrix approach with least-squares weighting functions up to an infinite truncation parameter N, i.e., we would be able to perform the necessary inversion of the infinite matrix $\mathbf{A}_{\partial\Gamma}$ in (68), for example. But this definition is of less importance for practitioners since one can find no clear answer whether the outgoing plane wave functions form a Schauder basis on a sinusoidal surface or not. And if they do this would be of little help since every numerical procedure is based in principle on a finite numerical accuracy and on a finite series expansion, and it has to fight against stability problems like the bad condition number of major matrices one has to invert in the process of the numerical solution.

2.5. Lippmann's criticism and the corresponding approach

Lippmann's criticism of Rayleigh's approach is much more intuitive and traceable for practitioners since it is based on the clear physical picture of Huygens' principle, at first glance (see Fig. 4). It is therefore used very often in recent papers as a justification for the supposed advantage of boundary integral equation methods and can be formulated as follows:

For observation points above the line $y = h$ Lippmann agrees with Rayleigh's representation of the scattered field as a series expansion in terms of outgoing waves only. But in observation points below $y = h$ there exist surface current elements generating waves which moves toward the surface of the grating. Ignoring those waves will result in an incomplete method to calculate the scattered field.

If we speak about Rayleigh's hypothesis in this subsection we have this understanding of Lippmann in mind. It is not easy to withstand his argumentation. Applying it to our Green's function formalism means that representations (60) and (57) are not allowed

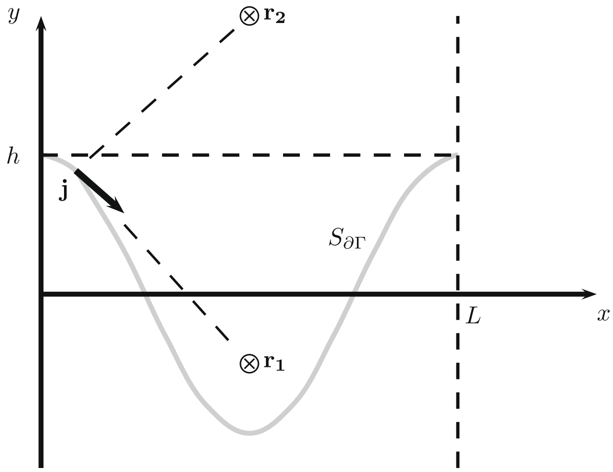

Fig. 4. Lippmann's criticism on Rayleigh's approach is based on the assumption that in point $\mathbf{r}_1$ also waves must be taken into account which moves toward the surface of the grating. These waves stem from surface current elements j above $\mathbf{r}_1$.

in the grooves of the grating. Or, in other words, replacing $\widetilde{G}_0(\mathbf{r},\hat{\mathbf{r}})$ in the surface integral of (52) by $\widetilde{G}_0^{>}(\mathbf{r},\hat{\mathbf{r}})$ is not allowed for points in the grooves up to the surface $R(x)$. This point of view seems to be even more supported by the fact that according to (35) series expansion (36) is a valid representation of the free-space Green's function in (60) only if $y > \hat{y}$. But this replacement was the essential step to derive the T-matrices. Fortunately, beside his pure criticism, Lippmann provided a loophole. Using the full free-space Green's function, i.e., employing Eq. (52) instead of (55) in the grooves up to the surface will not suffer from his criticism. This will lead us to a boundary integral equation with part of its kernel exhibiting a logarithmic singularity. As we have already mentioned in chapter 2.2.1 this singularity is not obvious in representation (21) or (34), respectively. There exists an equivalent representation which shows this singularity more clearly. It is given by

$$G_0(\mathbf{r},\mathbf{r}') = -\frac{i}{4}\cdot\sum_{n=-\infty}^{\infty} H_0^{(1)}(k_0 r_n);$$
$$r_n = \sqrt{(x - x' - nL)^2 + (y - y')^2} \tag{85}$$

with $H_0^{(1)}$ being the Hankel function of zero order and first kind [22]. Please, note that this representation contains both even and odd parts with respect to x. Since the logarithmic singularity is a weak singularity the calculation of the surface integral for p-polarized waves provides no difficulties (the case of s-polarized waves which can be related to the von Neumann problem is a little bit more complicate and can be treated by using Maue's boundary integral equation as described in [5,31], for example). But it should be pointed out already that both representations provide the same numerical results. Therefore we will use (34) in the subsequent analysis. $W^L_{\partial\Gamma}$ can then be calculated from

$$G^L_+(\mathbf{r},\mathbf{r}') = \widetilde{G}_0^{<}(\mathbf{r},\mathbf{r}') + \int_{S_{\partial\Gamma}} \widetilde{G}_0(\mathbf{r},\hat{\mathbf{r}})\cdot W^L_{\partial\Gamma}(\hat{\mathbf{r}},\tilde{\mathbf{r}}) \cdot \widetilde{G}_0^{<}(\tilde{\mathbf{r}},\mathbf{r}')dS(\hat{\mathbf{r}})dS(\tilde{\mathbf{r}}) \tag{86}$$

in the following way:

The interaction operator will be approximated by the bilinear expansion

$$W^L_{\partial\Gamma}(\hat{\mathbf{r}},\tilde{\mathbf{r}}) = \frac{i}{2L}\cdot\sum_{n,n'=0}^{N}\chi_n(\hat{\mathbf{r}})\cdot[\Omega^L_{\partial\Gamma}]_{n,n'}\cdot\chi^*_{n'}(\tilde{\mathbf{r}});\quad \hat{\mathbf{r}},\tilde{\mathbf{r}}\in S_{\partial\Gamma} \tag{87}$$

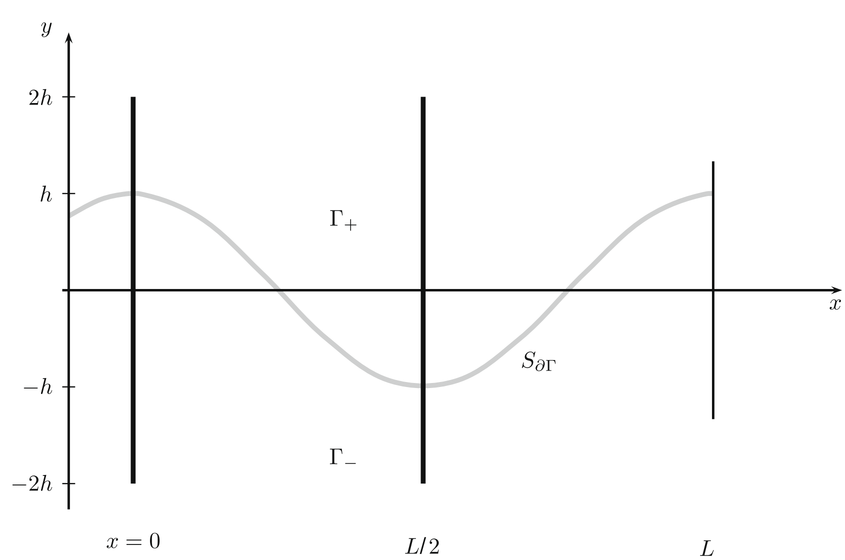

Fig. 5. The scattered field is plotted along the line $x = 0$ in Figs. 6, 9, and 12, and along the line $x = L/2$ in Figs. 7, 10, and 13. To verify the boundary condition the scattered field is additionally plotted in Figs. 8 and 11 along the boundary surface $S_{\partial\Gamma}$.

with expansion functions $\chi_n(x,R(x))$ given by

$$\chi_n(x,R(x)) = \frac{\tilde{\phi}_n(x,R(x))}{S(x)}. \tag{88}$$

The denominator $S(x)$ is defined in Eq. (54). If we insert this bilinear expansion and series expansion (37) (which is now again assumed to be finite!) into (86) we get from boundary condition (44)

$$\begin{aligned}
&-\frac{i}{2L}\sum_{m'=0}^{N}\tilde{\psi}_{m'}(x,R(x))\cdot\tilde{\phi}_{m'}(\mathbf{r}')\\
&= \left(\frac{i}{2L}\right)^2\sum_{n,n',m'=0}^{N}\int_{S_{\partial\Gamma}}\widetilde{G}_0(x,R(x);\hat{\mathbf{r}})\,\frac{\tilde{\phi}_n(\hat{\mathbf{r}})}{S(\hat{\mathbf{r}})}\cdot[\Omega^L_{\partial\Gamma}]_{n,n'}\cdot\frac{\tilde{\phi}^*_{n'}(\tilde{\mathbf{r}})}{S(\tilde{\mathbf{r}})}\\
&\quad\cdot\tilde{\psi}_{m'}(\tilde{\mathbf{r}})dS(\hat{\mathbf{r}})dS(\tilde{\mathbf{r}})\cdot\tilde{\phi}_{m'}(\mathbf{r}')\\
&= -\frac{1}{4L}\sum\nolimits_{n,n',m'=0}^{N}\int_0^L\widetilde{G}_0(x,R(x);\hat{x},R(\hat{x}))\cdot\tilde{\phi}_n(\hat{x},R(\hat{x}))d\hat{x}[\Omega^L_{\partial\Gamma}]_{n,n'}\\
&\quad\cdot[B^{(\tilde{\phi},\tilde{\psi})}_{\partial\Gamma}]_{n',m'}\cdot\tilde{\phi}_{m'}(\mathbf{r}').
\end{aligned}\tag{89}$$

The matrix elements $[B^{(\tilde{\phi},\tilde{\psi})}_{\partial\Gamma}]_{n',m'}$ are defined according to (66)/(67). Next we multiply this equation with $\tilde{\phi}^*_m(x,R(x))$ and integrate over x. This provides

$$\begin{aligned}
\sum\nolimits_{m'}[B^{(\tilde{\phi},\tilde{\psi})}_{\partial\Gamma}]_{m,m'}\cdot\tilde{\phi}_{m'}(\mathbf{r}') &= -\frac{i}{2}\sum_{n,n',m'}[\widetilde{G}^{(\tilde{\phi},\tilde{\phi})}_{\partial\Gamma}]_{m,n}\cdot[\Omega^L_{\partial\Gamma}]_{n,n'}\\
&\quad\cdot[B^{(\tilde{\phi},\tilde{\psi})}_{\partial\Gamma}]_{n',m'}\cdot\tilde{\phi}_{m'}(\mathbf{r}')
\end{aligned}\tag{90}$$

with

$$\begin{aligned}
[\widetilde{G}^{(\tilde{\phi},\tilde{\phi})}_{\partial\Gamma}]_{m,n} &= \frac{1}{L}\int_0^L\tilde{\phi}^*_m(x,R(x))\cdot\widetilde{G}_0(x,R(x);\hat{x},R(\hat{x}))\\
&\quad\cdot\tilde{\phi}_n(\hat{x},R(\hat{x}))dxd\hat{x}.
\end{aligned}\tag{91}$$

As already mentioned the calculation of this integral provides no difficulties independent of whether representation (34) or (85) is used. Thus we have finally the equation system (in matrix notation)

$$\mathbf{B}^{(\tilde{\phi},\tilde{\psi})}_{\partial\Gamma} = -\frac{i}{2}\cdot\widetilde{G}^{(\tilde{\phi},\tilde{\phi})}_{\partial\Gamma}\cdot\mathbf{\Omega}^L_{\partial\Gamma}\cdot\mathbf{B}^{(\tilde{\phi},\tilde{\psi})}_{\partial\Gamma} \tag{92}$$

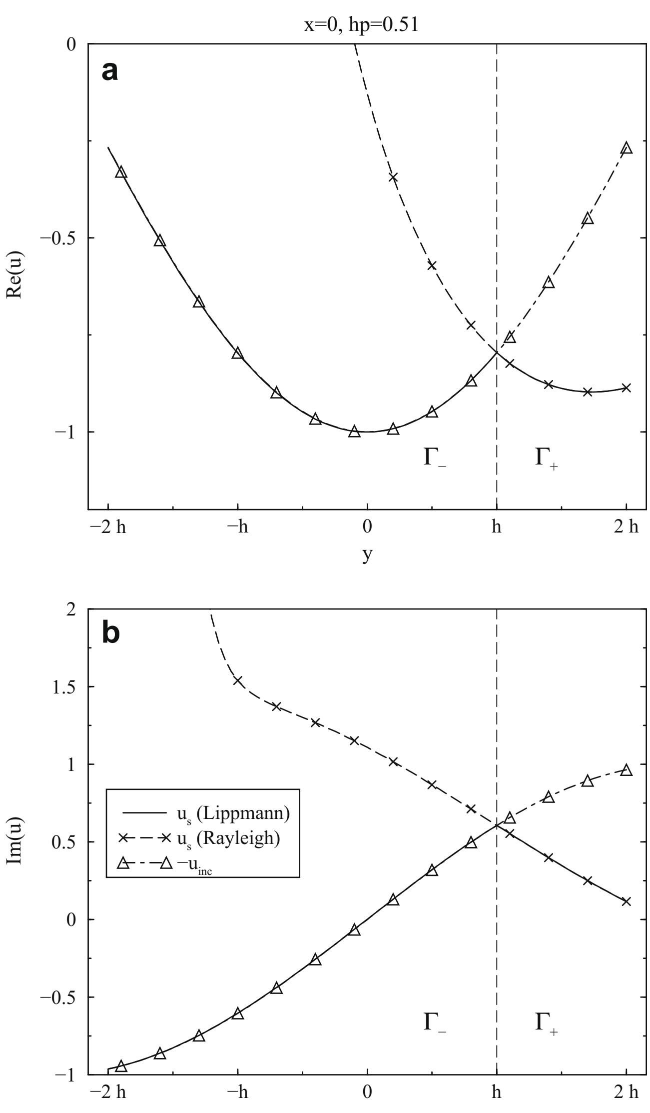

Fig. 6. Fields $u_s(x,y)$ and $-u_{inc}(x,y)$ (real part in (a), imaginary part in (b)) for $h\cdot p = 0.51$ ($k_0 = 1$, $L = 8$ and $h = 0.65$) along the line $x = 0$. For the Lippmann approximation of u_s (solid line) $N = 10$, and for the Rayleigh approximation (dashed line with crosses) $N = 18$ was used. $-u_{inc}$ (dot-dashed line with triangles) is also plotted for comparison.

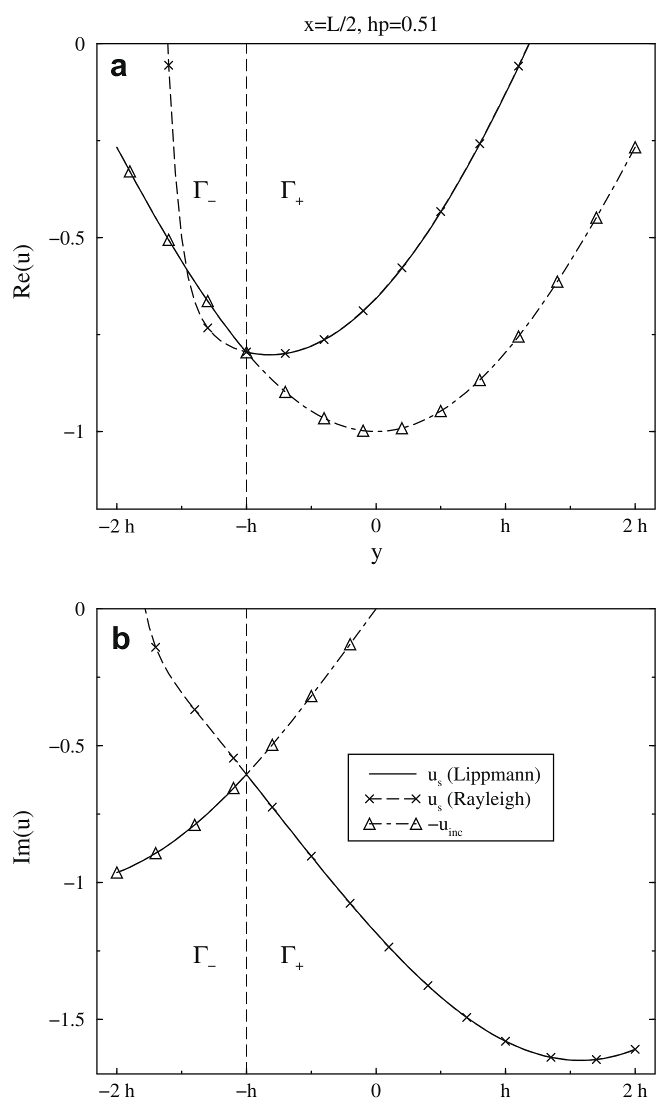

Fig. 7. Fields $u_s(x,y)$ and $-u_{inc}(x,y)$ (real part in (a), imaginary part in (b)) for $h\cdot p = 0.51$ along the line $x = L/2$. The same parameters as in Fig. 6 are used.

from which we can determine $\mathbf{\Omega}^L_{\partial\Gamma}$ according to

$$\mathbf{\Omega}^L_{\partial\Gamma} = 2i[\widetilde{\mathbf{G}}^{(\tilde{\phi},\tilde{\phi})}_{\partial\Gamma}]^{-1}. \tag{93}$$

$$G^L_+(\mathbf{r},\mathbf{r}') = \widetilde{G}^<_0(\mathbf{r},\mathbf{r}') - \frac{i}{2L}\sum_{n,n',m'=0}^{N}\int_0^L \widetilde{G}_0(\mathbf{r},\hat{\mathbf{r}})\cdot\tilde{\phi}_n(\hat{r})d\hat{x} \cdot [\widetilde{G}^{(\tilde{\phi},\tilde{\phi})^{-1}}_{\partial\Gamma}]_{n,n'}\cdot[B^{(\tilde{\phi},\tilde{\psi})}_{\partial\Gamma}]_{n',m'}\cdot\tilde{\phi}_{m'}(\mathbf{r}') \tag{94}$$

and

$$u_s(\mathbf{r}) = -\sqrt{k_0}\sum_{n,n'=0}^{N}\int_0^L \widetilde{G}_0(\mathbf{r},\hat{\mathbf{r}})\cdot\tilde{\phi}_n(\hat{r})d\hat{x}\cdot[\widetilde{G}^{(\tilde{\phi},\tilde{\phi})^{-1}}_{\partial\Gamma}]_{n,n'}\cdot[B^{(\tilde{\phi},\tilde{\psi})}_{\partial\Gamma}]_{n',0} \tag{95}$$

are the corresponding expressions for the Green's function and for the scattered field in Γ_+ we are interested in.

According to Lippmann's argumentation there should be a difference between representation (14) with coefficients calculated according to (59)/(68), and representation (95) of the scattered field especially within the grooves of the grating. If this really happens will be discussed in the final chapter.

3. Numerical considerations

Even if Millar has already demonstrated with his proof that outgoing plane waves form a complete system of functions on a sinusoidal surface there remains an uncertain feeling, and the impact of Lippmann's argumentation of the incompleteness of only outgoing waves within the grooves can still be observed also in the recent literature dealing with the numerical analysis of gratings. The goals of our numerical considerations are therefore the following:

- We want to demonstrate essentially that there is **no difference** in the numerical results between the T-matrix approach with weighting functions according to (70) and (74), and the approach (95) based on Lippmann's argumentation even in the grooves of the grating, and even beyond the found groove depth limit for conventional point-matching procedures.
- We want to demonstrate that Rayleigh's original approach with weighting functions which does not belong to a least-squares scheme is able to produce accurate results even in the grooves also if $h \cdot p$ exceeds the value of 0.448. The obtained results agree with the approach based on Lippmann's argumentation.

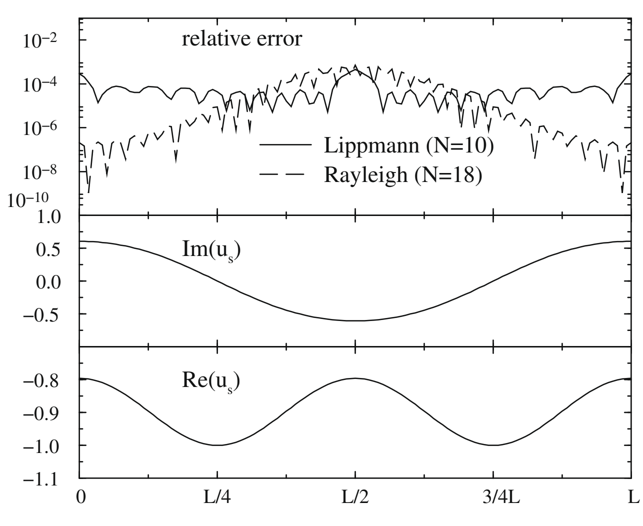

Fig. 8. Lippmann's and Rayleigh's approximation of the scattering field $u_s(x,R(x))$ for $h \cdot p = 0.51$ along the surface $S_{\partial\Gamma}$ (parameters: see Fig. 6). The relative error is calculated according to $|u_s(x,R(x)) + u_{inc}(x,R(x))|/|u_{inc}(x,R(x))|$.

- In close connection to this we want to demonstrate that not only least-squares schemes are able to exceed numerically the upper limit $h \cdot p = 0.448$.
- We want to demonstrate that the solution scheme based on Lippmann's argumentation does not provide an analytical solution at the surface of the grating as it should be since the normal derivative of the electric field exhibit a jump at the surface which is related to the induced surface current. Below the surface it cancels the primary incident plane wave, as expected. The T-matrix approach, on the other hand, results in a representation which is continuous across the surface but becomes divergent somewhere below the surface. The latter is of course meaningless for practical applications since the corresponding representation of the scattered field holds only above the grating and on its surface.

For these purposes we have plotted the scattered field data of the different approaches along the two lines depicted in Fig. 5 as well as along the surface of the grating. The latter was done to

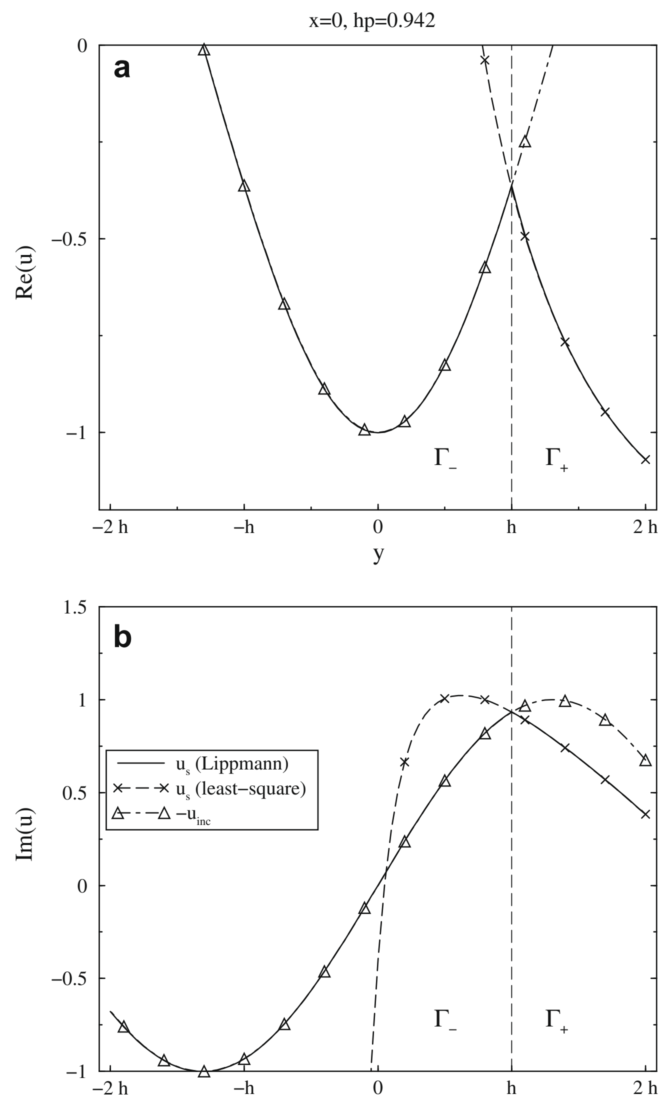

Fig. 9. Fields $u_s(x,y)$ and $-u_{inc}(x,y)$ (real part in (a), imaginary part in (b)) for $h \cdot p = 0.942$ ($k_0 = 1$, $L = 8$ and $h = 1.2$) along the line $x = 0$. For the Lippmann approximation of u_s (solid line) $N = 12$, and for the least-squares approximation (dashed line with crosses) $N = 18$ was used. $-u_{inc}$ (dot-dashed line with triangles) is also plotted for comparison.

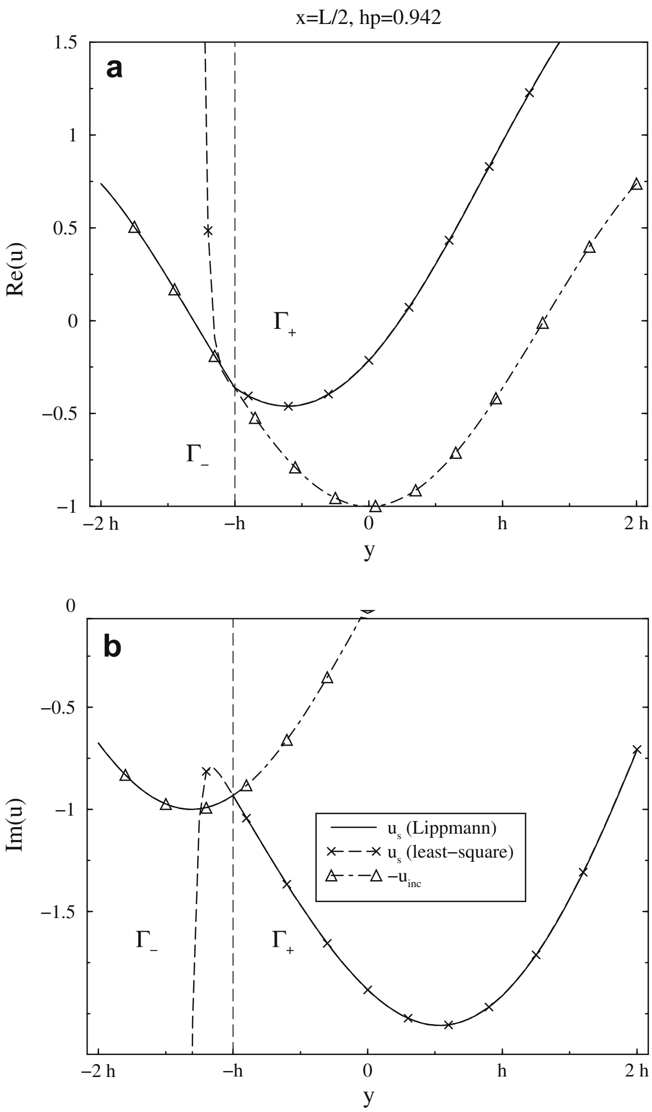

Fig. 10. Fields $u_s(x,y)$ and $-u_{inc}(x,y)$ (real part in (a), imaginary part in (b)) for $h \cdot p = 0.942$ along the line $x = L/2$. The same parameters as in Fig. 9 are used.

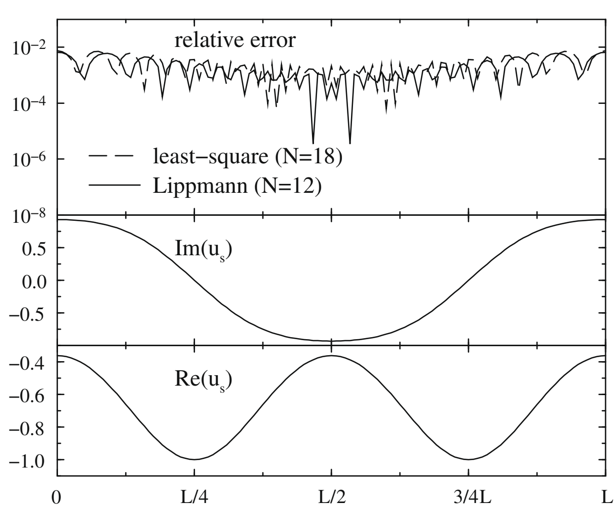

Fig. 11. Lippmann's and Rayleigh's approximation of the scattering field $u_s(x,R(x))$ for $h \cdot p = 0.942$ along the surface $S_{\partial\Gamma}$ (parameters: see Fig. 9). The relative error is calculated according to $|u_s(x,R(x)) + u_{inc}(x,R(x))|/|u_{inc}(x,R(x))|$.

demonstrate the fulfilment of the boundary condition. The truncation parameter N and the number of expansion terms used to represent the free-space Green's function in all of our calculations was chosen according to the requirement that the relative error of this boundary condition does not exceed 1% along the whole surface. Concerning the boundary integral equation approach we have to fix additionally the accuracy of the surface integration which must be performed numerically, and the number of expansion terms used in the representation of the full free-space Green's function $\widetilde{G}_0$. To calculate (91) we used a two-dimensional Gauss-Kronrod formula with a step width ensuring a relative error less than 10^{-3}. The same was done to calculate the scattered field according to (95) but with an one-dimensional Gauss-Konrod formula. The number of expansion terms in the representation of $\widetilde{G}_0$ was the most sensitive parameter in these calculations. If $h \cdot p = 0.51$ was chosen it was necessary to take 200 expansion terms into account. $h \cdot p = 0.942$ required 300 expansion terms to achieve the above mentioned accuracy of the boundary condition. A standard NAG routine was used for the necessary matrix inversion. All calculations have been performed with double precision accuracy.

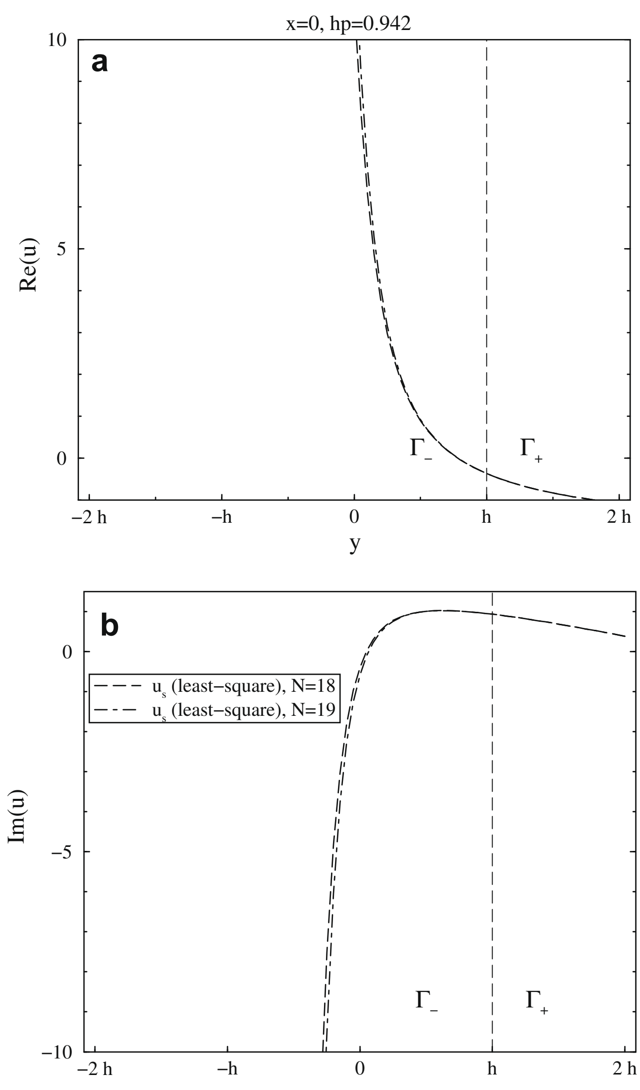

Fig. 12. Least-square approximations of u_s at $h \cdot p = 0.942$ (see Fig. 9 for details) for two consecutive truncation parameters N along the line $x = 0$ ($N = 18$ – dashed, $N = 19$ – dot-dashed).

All relevant parameters can be found in the figure captions. Figs. 6–8 demonstrate the excellent agreement between Rayleigh's original approach and the boundary integral equation approach even if $h \cdot p$ exceeds the limit of 0.448. Moreover it can be clearly seen that in Γ_- the result of the boundary integral equation approach cancles the incident plane wave. The least-squares approach based on the weighting functions (74) produces in Γ_+ and at the surface of the grating results which cannot be distinguished from Rayleigh's approach but for a lower truncation parameter N ($N = 10$ in this case). If $h \cdot p = 0.942$ is considered no convergence could be achieved with Rayleigh's approach but with the least-squares method. The results of the latter are plotted in Figs. 9–11 against the results obtained with the boundary integral equation method. We can state again an excellent agreement. In Figs. 12 and 13 it is shown that the series expansion of the scattered field based on the T-matrix approach with the least-squares weighting functions seems to diverge in Γ_- but at different locations along the lines $x = 0$ and $x = L/2$. It should be mentioned that it is more difficult to achieve convergence in the near-field than for the scattering quantities in the far-field. $h \cdot p = 0.942$ was the upper limit we could obtain within double precision accuracy for the above mentioned criterion of the fulfilment of the boundary condition.

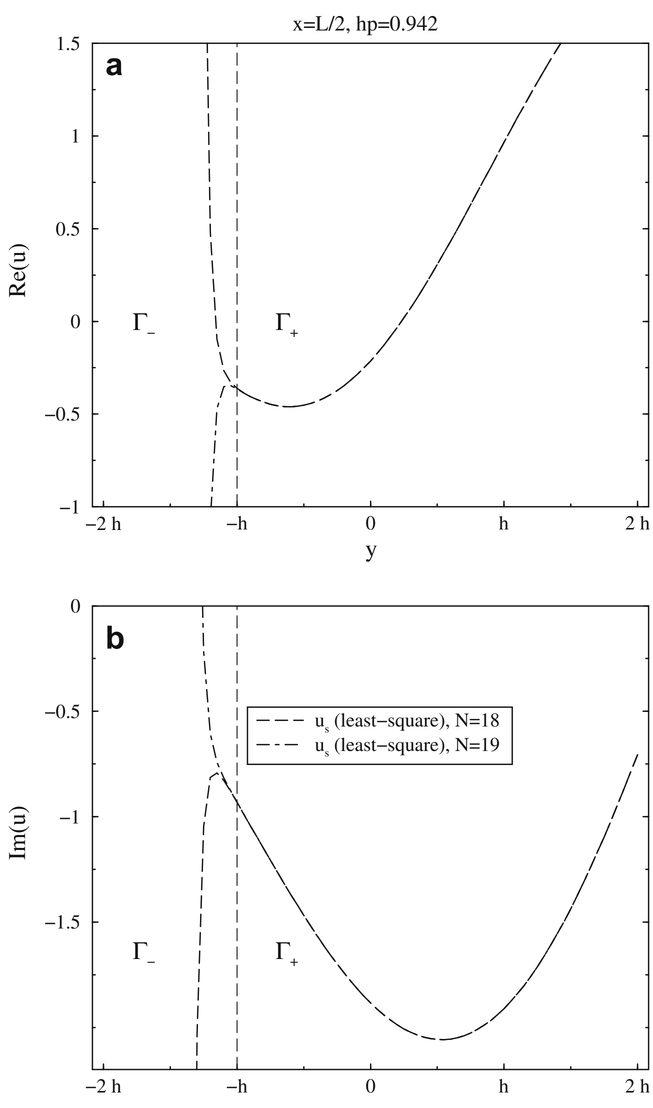

Fig. 13. Least-square approximations of u_s at $h \cdot p = 0.942$ (see Fig. 9 for details) for two consecutive truncation parameters N along the line $x = L/2$ ($N = 18$ – dashed, $N = 19$ – dot-dashed).

4. Conclusion

In this paper we have presented a rigorous Green's function formulation of the problem of plane wave scattering from a perfectly conducting and sinusoidal surface. The considerations have been restricted to a perpendicular incident and p-polarized plane wave. Based on this scattering problem the different point of views on Rayleigh's hypothesis have been discussed. It was demonstrated that there are especially two different understandings which can be related to two different formulations of Huygens' principle in terms of Green's functions resulting in two different expressions for the corresponding interaction operators. One formulation results in the T-matrix approach with the additional degree of freedom to chose appropriate weighting functions. The other formulation is equivalent to boundary integral equation approaches.

Concerning T-matrix methods there is only a general problem according to Petit, Cadilhac, and Millar if the delta distributions are taken as weighting functions in such a way that one gets conventional point-matching. But this is of less interest in practical applications due to the instabilities of such a procedure. Generalized point-matching methods or T-matrix approaches with other weighting functions (including Rayleigh's original approach) are more appropriate. The presented numerical results and their intercomparison with the results obtained by use of a certain boundary integral equation method suggest that T-matrices can be used for near-field calculations also beyond the theoretical groove depth limit discussed in the context of Rayleigh's hypothesis.

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