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# Rapidly convergent two-dimensional quasi-periodic Green function throughout the spectrum—including Wood anomalies



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#### ABSTRACT

We introduce a new methodology, based on new quasi-periodic Green functions which converge rapidly even at and around Wood-anomaly configurations, for the numerical solution of problems of scattering by periodic rough surfaces in two-dimensional space. As is well known the classical quasi-periodic Green function ceases to exist at Wood anomalies. The approach introduced in this text produces fast Green function convergence throughout the spectrum on the basis of a certain "finite-differencing" approach and smooth windowing of the classical Green function lattice sum. The resulting Green-function convergence is super-algebraically fast away from Wood anomalies, and it reduces to an arbitrarily-high (user-prescribed) algebraic order of convergence at Wood anomalies.

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#### 1. Introduction

We consider the problem of evaluation of the fields scattered by a periodic perfectly conducting surface under plane-wave illumination. This problem has been extensively studied as it impacts upon a wide range of areas of science and engineering, including optics, photonics, communications, and stealth, and, through them, many fields of physics, astronomy, chemistry, biology and metallurgy [30,44]. A variety of numerical approaches have been used to tackle this important problem [10,30,38,42] including, notably, methods based on use of integral equations [33]. Recent integral equation methods [6,7], in particular, have made it possible to obtain, in reasonable computing times, highly accurate solutions for very challenging problems of scattering by periodic surfaces. The success of this methodology lies in part on its inherent dimensionality reduction (only the scattering surface needs to be discretized, not the surrounding volume) and associated automatic enforcement of radiation conditions; mathematical analyses of the integral equation method in various contexts, including scattering by periodic surfaces and bounded obstacles, can be found in [1,9,15,17,23,33,42] and references therein.

The properties of integral equations for periodic surfaces under plane-wave incidence are closely related to the character of the corresponding quasi-periodic Green functions used. As is well known, classical expressions for quasi-periodic Green functions converge extremely slowly, and a number of methods have therefore been introduced to produce rapidly convergent Green-function algorithms, including the well known Ewald summation method [2,12,27] for two- and

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three-dimensional problems and, for the two-dimensional case, the highly efficient algorithm [45]. Many other contributions have in fact been put forward over the years to facilitate evaluation of quasi-periodic Green functions; in addition to those mentioned above here we mention [13,18,24,32,36,39,40]; a recent survey can be found in [29]. A combined approach which takes advantage of various methods, applying each algorithm for configurations for which it is most efficient (for the challenging three-dimensional Green function problem), was put forth in [20].

As is well known, none of these methods for evaluation of the quasi-periodic Green function can be applied to problems of scattering by periodic surfaces at Wood-anomaly configurations [43,46] (at which one or more scattered waves propagate in a direction parallel to the scattering surface): for Wood-anomaly configurations the classical periodic Green function is not even defined (see Remark 2.2 for details on nomenclature concerning Wood anomalies). To address this difficulty we propose new quasi-periodic Green functions and associated series representation which converge rapidly even at and around Wood anomalies. More precisely, we present a set of rapidly convergent quasi-periodic Green functions  $G_j^q$  whose *N*-term truncated series converge, at Wood anomalies, at least as fast as  $(1/N)^{(j-1)/2}$  for j even (resp.  $(1/N)^{j/2}$  for j odd) as  $N \to \infty$ ; in view of the fact that this approach also incorporates the smooth windowing function methodology [35], the new Green functions also enjoy super-algebraically fast convergence (faster than any power of N) away from Wood anomalies.

The approach introduced in this text produces fast Green-function convergence at and around Wood anomalies on the basis of a certain order-j "finite-differencing" method (for positive integer values of j). To our knowledge, this is the first approach ever presented that is applicable to problems of scattering by diffraction gratings at Wood anomalies on the basis of quasi-periodic Green functions.

It should be noted that a "method-of-images Green-function", which is related to our j=1 Green function approach, was used in [14,47] to treat problems of scattering by nonlocal, non-periodic perturbations of a line in two dimensions. The j=1 method, which suffices to yield (slow) convergence in the two-dimensional case, does not give rise to convergence in three dimensions: for three-dimensional configurations convergence only results for  $j \ge 2$  [11]. In this context we also mention the recent work [3,4] which, for two-dimensional problems, introduces an alternative integral equation which does not utilize a quasi-periodic Green function, and which is also applicable at Wood anomalies: in that approach quasi-periodicity is enforced through use of auxiliary layer potentials on the periodic cell boundaries. The practical feasibility of an extension of this methodology to three-dimensional problems has not as yet been established.

In order to demonstrate the character of the new approach we present efficient numerical methods, based on the new Green functions, for the solution of quasi-periodic scattering problems throughout the spectrum—even at and around Wood anomalies—; as shown in Section 4.4, certain slight modifications of the direct finite-differencing Green function expressions mentioned above need to be introduced to obtain uniquely solvable integral-equation problems. We further mention that, as indicated in [11], additional acceleration can be induced in the Green-function convergence by means of the FFT-based equivalent-source methodology [8]; see Remark 6.2. Our numerical results demonstrate the capabilities of the new methodology: even in absence of the acceleration method [8,11], the present approach can solve the complete scattering problem for rather challenging periodic surfaces (steep gratings) in the resonance regime, including Green function computations and matrix inversion by means of Gaussian elimination, in total computing times of a few tens to a few hundreds of milliseconds—depending on the complexity of the problem.

The remainder of this paper is organized as follows. Section 2 describes the scattering problem under consideration and it presents some background on quasi-periodic function and integral equations. Section 3 describes the smooth windowing method that gives rise to super-algebraically converging Green function away from Wood anomalies. Section 4 then presents the new rapidly convergent Green functions together with necessary theoretical discussions involving the Green function itself and associated integral equations. Section 5 describes the numerical implementation of the new Green functions and integral equations, and Section 6, finally, presents a variety of numerical results demonstrating the properties of the overall proposed approach.

#### 2. Preliminaries

#### 2.1. Scattering problem

We consider the problem of scattering of a plane wave by a perfectly reflecting periodic surface

$$\Gamma = \{(x, f(x)), x \in \mathbb{R}\}$$

with  $f \in \mathcal{C}^r_{\text{per}}(\mathbb{R})$ ,  $r \geqslant 2$ , where, for any non-negative integer r,  $\mathcal{C}^r_{\text{per}}(\mathbb{R})$  denotes the set of L-periodic r-times continuously differentiable functions defined in the real line. The propagation domain is thus the region

$$\Omega = \{ (x, y) \in \mathbb{R}^2, \text{ such that } y > f(x) \}.$$
 (2)

Letting k be a positive wavenumber and, further, letting  $\theta \in (-\pi/2, \pi/2)$ ,  $\alpha = k \sin(\theta)$  and  $\beta = k \cos(\theta)$ , we assume the periodic surface is illuminated by the incident plane wave

$$u^{\text{inc}}(x,y) = e^{i(\alpha x - \beta y)} \tag{3}$$

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