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II: The three-dimensional scalar case

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ANALYSIS OF MULTIPLE SCATTERING ITERATIONS FOR HIGH-FREQUENCY SCATTERING PROBLEMS. II: THE THREE-DIMENSIONAL SCALAR CASE

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ABSTRACT. In this paper we continue our analysis of the treatment of multiple scattering effects within a recently proposed methodology, based on integral-equations, for the *rigorous* numerical solution of scattering problems at high frequencies. In more detail, here we extend the two-dimensional results in part I of this work to fully three-dimensional geometries. As in the former case, our concern here is the determination of the rate of convergence of the multiple-scattering iterations that are inherent in the aforementioned high-frequency schemes. To this end, we follow a similar strategy to that we devised in part I: first, we recast the (iterated, Neumann) multiple-scattering series in the form of a sum of *periodic orbits* (of increasing period) corresponding to multiple reflections that periodically bounce off a series of scattering sub-structures; then, we proceed to derive a high-frequency recurrence that relates the “currents” (i.e. the normal derivative of the fields) induced on these structures as the waves reflect periodically; and, finally, we analyze this recurrence to provide an *explicit* rate of convergence associated with each orbit. While the procedure is analogous to its two-dimensional counterpart, the actual analysis is significantly more involved and, perhaps more interestingly, it uncovers new phenomena that cannot be distinguished in two-dimensional configurations (e.g. the further dependence of the convergence rate on the relative *orientation* of interacting structures). As in the two-dimensional case, and beyond their intrinsic interest, we also explain here how the results of our analysis can be used to *accelerate* the convergence of the multiple-scattering series and, thus, to provide significant savings in computational times.

1. INTRODUCTION

This paper constitutes the second part in a series that seeks to analyze the convergence characteristics of multiple-scattering iterations within a recently proposed scheme for the numerical solution of high-frequency scattering problems [2, 3]. As we explained in part I of this series [6], which dealt with two-dimensional configurations, the methods in [2, 3] result from a set of ideas that collectively deliver a unique scattering solver, capable of predicting scattering returns within any *prescribed accuracy* in *frequency-independent* computational times. Here we extend the analysis in [6] to encompass fully three-dimensional configurations within scalar (e.g. acoustic) scattering models.

For a review on the relevance of these novel schemes for the simulation of high-frequency scattering scenarios, and for their placement in the context of state-of-the-art numerical procedures for scattering applications we refer the reader to [2, 3, 6]. As detailed therein, these new schemes overcome the classical limitations of alternative methods (namely, the need to numerically resolve the fields on the scale of the wavelength of radiation) while retaining their most important characteristics (e.g. error-controllability). As such, these novel numerical algorithms have generated significant interest and work in recent years (see e.g. [4, 8, 7]), which has been mostly confined to two-dimensional, single-scattering geometries (e.g. those that arise in connection with scattering by cylindrical convex obstacles).

Work on the implementation of the basic ideas in [2] for the treatment of fully three-dimensional configurations, on the other hand, reduces to the (single-scattering) results in [1]. As in the two-dimensional case, these results can be used to extend the methodology to cases wherein multiple-scattering occurs, following the prescriptions in [3]. More precisely, as we review in Sect. 2.3, the approach to the account of multiple-scattering effects relies on the reformulation of the integral-equation representation of the scattering problem in the form of an iterative series, whose terms can be derived from the sequential solution of single-scattering problems corresponding to successive geometrical reflections in the limit of infinite frequency. While the results in [1] provide clear guidelines for the attainment of a prescribed accuracy in the simulation of each of

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these single-scattering events (at arbitrarily high frequencies), the question of convergence of the multiple-scattering series that they collectively constitute has remained unexplored. Here we provide an analysis of this convergence that is analogous to that we devised in [6] for the two-dimensional case.

In fact, the procedure we follow here to uncover the convergence characteristics of the multiple-scattering series in three dimensions is similar to that we introduced in [6]. Specifically, the method is based on (i) a recasting of the iterated multiple-scattering series in the form of a sum of *periodic orbits* (of increasing period) corresponding to multiple reflections that periodically bounce off a series of scattering sub-structures (see Sect. 2.4); (ii) an analysis of these periodic orbits in the high-frequency regime which delivers a recurrence that relates the “currents” (i.e. the normal derivative of the fields) induced on the sub-structures as the waves reflect periodically (Sect. 3); and, (iii) a derivation that relies on (ii) to provide an *explicit* rate of convergence associated with each orbit (Sect. 4). Numerical results that exemplify the relevance and accuracy of these analytical developments are presented in Sect. 5.

While the approach we use here to establish our results in three dimensions is analogous that we utilized to prove their two-dimensional counterparts, the actual analyses are significantly more involved. To facilitate this comparison and the overall understanding of the results we present here, the rest of this paper is largely organized as the first part of the series [6], to which we refer throughout to minimize the repetition of arguments. In particular, for instance, a comparison of our main results (cf. [6, Theorems 3.1, 4.1, 4.2 and Corollary 4.14] and Theorems 3.1, 4.11, 4.13 and Corollary 4.14 below) clearly demonstrates the significant additional complexities that the extension to three space dimensions entails. More interestingly, perhaps, this extension uncovers new phenomena that cannot be distinguished in two-dimensional configurations, such as the further dependence of the convergence rate on the relative *orientation* of interacting structures (see, e.g., Theorem 4.11, Remark 4.12 and Tables 2–3).

Finally, as in the two-dimensional case, and beyond their relevance in providing an error estimate for any truncation of the multiple-scattering series, the results of our analysis can be further used to *accelerate* the convergence of this series and, thus, to provide significant savings in computational times. As explained in [6, Sect. 5.2], this acceleration can be attained in a number of ways. For instance, knowledge of the asymptotic behavior of the terms in the series as the number of reflections increases, allows for an extrapolation of the neglected tail which can be added to a numerically evaluated series, truncated at any given order, to deliver a more accurate estimate of the overall sum. Clearly, other acceleration strategies are possible (e.g. based on suitable *combinations* of the iterates —as done, for example, in classical methodologies based on Krylov subspaces—). The extension of our analysis to encompass these alternative techniques, as well as that corresponding to vector scattering models (e.g. the Maxwell system), however, are left for future work.

2. PRELIMINARIES

In this section we collect some preliminary results that will provide the framework for the developments that follow. We begin with a statement of the scattering problem and recall its integral equation formulation. We then review some recently introduced methods for its solution at high frequencies that incorporate multiple scattering effects; finally, we show that these effects can be fully accounted for through consideration of periodic orbits.

2.1. The scattering problem and integral equations. We consider the problem of evaluating the scattering of an incident acoustic plane wave $u^{\text{inc}}(x) = e^{ik\alpha \cdot x}$, $|\alpha| = 1$, from a smooth impenetrable obstacle K . Throughout this paper we concentrate on three-dimensional configurations for which the relevant (frequency-domain) problem is modeled by the scalar Helmholtz equation

$$(2.1) \quad \Delta u(x) + k^2 u(x) = 0, \quad x \in \Omega = \mathbb{R}^3 \setminus \overline{K},$$

where the scattered field u is required to satisfy the Sommerfeld radiation condition

$$(2.2) \quad \lim_{|x| \rightarrow \infty} |x| \left[\left(\frac{x}{|x|}, \nabla u(x) \right) - ik u(x) \right] = 0.$$

For definiteness, we assume Dirichlet conditions on the boundary of the scatterer K

$$(2.3) \quad u(x) = -u^{\text{inc}}(x) = -e^{ik\alpha \cdot x}, \quad x \in \partial K.$$

As will be clear from the derivations that follow, extensions to other boundary conditions are rather straightforward.

The problem (2.1)–(2.3) can be recast in the form of an integral equation in a variety of ways (see e.g. [5]). For our purposes, a most convenient form is that derived from the Green identities

$$(2.4) \quad -u(x) = \int_{\partial K} \left(\frac{\partial u(y)}{\partial \nu(y)} \Phi(x, y) - u(y) \frac{\partial \Phi(x, y)}{\partial \nu(y)} \right) ds(y)$$

and

$$(2.5) \quad 0 = \int_{\partial K} \left(\frac{\partial u^{\text{inc}}(y)}{\partial \nu(y)} \Phi(x, y) - u^{\text{inc}}(y) \frac{\partial \Phi(x, y)}{\partial \nu(y)} \right) ds(y)$$

valid for all $x \in \Omega$, where $\nu(y)$ denotes the vector normal to ∂K and exterior to K , and

$$\Phi(x, y) = \frac{1}{4\pi} \frac{e^{ik|x-y|}}{|x-y|}$$

is the *outgoing* Green function. Adding (2.4) and (2.5), and using (2.3), it follows that

$$(2.6) \quad u(x) = - \int_{\partial K} \Phi(x, y) \eta(y) ds(y), \quad x \in \Omega,$$

where

$$(2.7) \quad \eta(y) = \frac{\partial (u(y) + u^{\text{inc}}(y))}{\partial \nu(y)}$$

represents the total induced current in the electromagnetic case. Using (2.6), (2.7) and the jump relations for the derivatives of single-layer potentials [5] we obtain the second-kind integral equation

$$(2.8) \quad \eta(x) - \int_{\partial K} \frac{\partial G(x, y)}{\partial \nu(x)} \eta(y) ds(y) = 2 \frac{\partial u^{\text{inc}}}{\partial \nu}(x), \quad x \in \partial K$$

for the unknown current η , where we have set $G = -2\Phi$. The solution of the integral equation (2.8) is not unique when the wavenumber k is an internal resonance and thus, in practical implementations, a “combined field” integral equation (CFIE) formulation is traditionally used [5]. However, the ideas that follow clearly extend to the CFIE formulation and thus, for the sake of simplicity in presentation, we shall assume that the wave number k is not an internal resonance and work with the integral equation (2.8).

2.2. High-frequency integral-equation method: single scattering [2]. As recognized in [2, 3], the advantages of (2.8) over alternative formulations (e.g. such as those based on the “indirect approach” [5]) in the numerical simulation of high-frequency applications stem from the physical nature of the unknown density η . Indeed, in the absence of multiple scattering, physical considerations suggest that the actual current should oscillate in-sync with the incident radiation, which allows for the *pre-determination* of its phase. More precisely, in this case, the current admits a factorization

$$(2.9) \quad \eta(x) = \eta^{\text{slow}}(x) e^{ik\alpha \cdot x},$$

where η^{slow} is “slowly oscillatory”, that is, its variations do not accentuate with increasing frequency and, therefore, its numerical approximation demands a significantly reduced number of degrees of freedom. In fact, in case K is convex, a very precise form of (2.9) has been shown to hold [10], which provides accurate descriptions for the behavior of the slow envelope in the illuminated and shadow regions

$$(2.10) \quad \partial K^{IL} = \{x \in \partial K : \alpha \cdot \nu(x) < 0\}$$

$$(2.11) \quad \partial K^{SR} = \{x \in \partial K : \alpha \cdot \nu(x) > 0\},$$

and for the transition between these through the shadow boundaries

$$\partial K^{SB} = \{x \in \partial K : \alpha \cdot \nu(x) = 0\}.$$

Theorem 2.1 ([10]). *If K is convex then, for all $P, Q \geq 0$, the current η^{slow} admits the representation*

$$(2.12) \quad \eta^{\text{slow}}(x) = \eta^{\text{slow}}(x, k, \alpha) = \sum_{p=0}^P \sum_{q=0}^Q k^{2/3-2p/3-q} b_{p,q}(\alpha, x) \Psi^{(p)}(k^{1/3} Z(\alpha, x)) + R_{P,Q}(k, \alpha, x)$$

where the complex-valued functions $b_{p,q}$ and the real-valued function Z are smooth, and Ψ is entire in the complex plane. Moreover, Z is positive in the illuminated region, negative in the shadow region, and vanishes precisely to first order at the shadow boundary. The function Ψ behaves asymptotically as

$$(2.13) \quad \Psi(\tau) = \begin{cases} \sum_{p=0}^n a_p \tau^{1-3p} + \mathcal{O}(\tau^{1-3(n+1)}) & \text{as } \tau \rightarrow \infty, \\ c_0 e^{-i\tau^3/3 - i\tau\beta} (1 + \mathcal{O}(e^{\tau c_1})) & \text{as } \tau \rightarrow -\infty, \end{cases}$$

for some constants c_0 and $c_1 > 0$, where $\beta = e^{-2\pi i/3} \beta_1$ and β_1 is the right-most root of Ai. The remainder $R_{P,Q}$ satisfies

$$|D_x^\gamma R_{P,Q}(k, \alpha, x)| \leq C_{P,Q,\gamma} (1+k)^{-\min\{2P/3, Q+1/3\} + 1/3|\gamma|}$$

for some constants $C_{P,Q,\gamma}$.

As was shown in [2], the representations (2.9), (2.12) can be used as the basis for an efficient (spectral) numerical scheme for the solution of the scattering problem, which can deliver answers within any prescribed accuracy in frequency-independent computational times. The procedure is based on the determination of the slow envelope η^{slow} which, from (2.8) and (2.9) clearly solves

$$(2.14) \quad \eta^{\text{slow}}(x) - \int_{\partial K} \frac{\partial G(x, y)}{\partial \nu(x)} e^{ik\alpha \cdot (y-x)} \eta^{\text{slow}}(y) ds(y) = 2ik\alpha \cdot \nu(x), \quad x \in \partial K.$$

The method of [2] relies on the iterative solution of a discretized version of (2.14), which reduces the problem to 1) the determination of an appropriate finite-dimensional representation of the unknown η^{slow} and 2) the design of an effective quadrature formula for the integral in the left-hand side. The expansion (2.12) provides the theoretical grounds to resolve the first problem: the discretization is chosen to be equispaced, and frequency-independent, in the illuminated region and it is refined in a neighborhood of the shadow boundaries to capture the corresponding boundary layers. In accordance with (2.12), this neighborhood covers a region of size proportional to $k^{-1/3}$, where the constant of proportionality is chosen so as to allow for the neglect, to within a desired accuracy, of the (exponentially small) contributions arising from the remaining, deep shadow region (cf. $\tau \rightarrow -\infty$ in (2.13)). Moreover, equation (2.13) guarantees that a *fixed*, frequency-independent number of points can be placed in these transition regions to obtain uniformly accurate solutions.

The integration scheme, on the other hand, is based on an error-controllable extension of the Method of Stationary Phase [9]. More precisely, the non-oscillatory nature of η^{slow} allows for the complete determination of the *phase* of the integrand in (2.14), namely

$$(2.15) \quad e^{ik\{\alpha \cdot (y-x) + |x-y|\}}$$

for each fixed value of the “target point” x . And, as shown in [2], this can be used to suitably *localize* the integral around *critical points* (i.e. singular points of the integrand, and stationary points of the phase), thereby enabling its evaluation in a fixed number of operations independently of k .

2.3. High-frequency integral-equation method: multiple scattering [3]. As is clear from the preceding discussion, a factorization of the form (2.9) is crucial in allowing for an efficient numerical solution of the integral equation (2.8) in the high-frequency regime. Evidently, in the presence of multiple-scattering the relation (2.9) is no longer valid. However, as suggested in [3], this relation possesses a natural extension to this case in the form

$$(2.16) \quad \eta(x) = \eta^{\text{slow}}(x) e^{ik\varphi(x)},$$

where φ corresponds to the solution of the asymptotic *geometrical optics* (GO) model, that is, to the solution of the eikonal equation.

Still, an additional problem arises in this case, as the solution $\varphi(x)$ will generally be multi-valued. On the other hand, these multiple values correspond precisely to successive wave reflections which suggests that they may be amenable to a sequential treatment. As was shown in [3], this is indeed possible if the integral

equation (2.8) is suitably reformulated. To review this (with a view to our analysis of the iterations in Sects. 3 and 4), let us assume that the scatterer K is decomposed into a collection of finitely many disjoint sets $K = \bigcup_{\sigma \in \mathcal{I}} K_\sigma$. Then, the integral equation (2.8) can be written as

$$(2.17) \quad (I - R)\eta = f$$

where $\eta(x) = (\eta_{\sigma_1}(x), \dots, \eta_{\sigma_{|\mathcal{I}|}}(x))^t$ and $f(x) = (f_{\sigma_1}(x), \dots, f_{\sigma_{|\mathcal{I}|}}(x))^t$ with η_σ and f_σ defined on K_σ and

$$f_\sigma(x) = 2ike^{ik\alpha \cdot x} \alpha \cdot \nu_\sigma(x) \quad \sigma \in \mathcal{I},$$

and the operator R is defined as

$$(2.18) \quad (R_{\sigma\tau}\eta_\tau)(x) = \int_{\partial K_\tau} \frac{\partial G(x, y)}{\partial \nu_\sigma(x)} \eta_\tau(y) ds(y) \quad \text{for } x \in K_\sigma.$$

Inverting the diagonal part of (2.17) yields the equivalent relation

$$(2.19) \quad (I - T)\eta = g$$

with

$$(2.20) \quad g_\sigma = (I - R_{\sigma\sigma})^{-1} f_\sigma, \quad \sigma \in \mathcal{I}$$

and

$$(2.21) \quad T_{\sigma\tau} = \begin{cases} (I - R_{\sigma\sigma})^{-1} R_{\sigma\tau} & \text{if } \sigma \neq \tau \\ 0 & \text{otherwise.} \end{cases}$$

As described in [3], the formulation (2.19) provides a convenient mechanism to account for multiple scattering since the n -th term in its Neumann series solution

$$(2.22) \quad \eta = \sum_{m=0}^{\infty} \eta^m = \sum_{m=0}^{\infty} T^m g$$

corresponds exactly to contributions arising as a result of waves that (in the high-frequency regime) have undergone n geometrical reflections. More precisely, we have

$$(2.23) \quad \eta^m|_{K_\sigma} = \sum_{\substack{\tau_0, \dots, \tau_{m-1} \in \mathcal{I} \\ \sigma \neq \tau_{m-1}, \tau_j \neq \tau_{j-1}}} T_{\sigma\tau_{m-1}} T_{\tau_{m-1}\tau_{m-2}} \cdots T_{\tau_1\tau_0} g_{\tau_0},$$

where each application of a $T_{\sigma\tau}$ entails an evaluation on K_σ of a field generated by a current on K_τ (cf. (2.18)), and its use as an incidence for a subsequent solution of a (single-)scattering problem on K_σ (corresponding to the inversion of $I - R_{\sigma\sigma}$ in (2.21)). In particular, this interpretation guarantees that for every path $(\tau_0, \dots, \tau_{m-1}, \tau_m)$ with $\tau_m = \sigma$ in (2.23) the geometrical phase is *uniquely* defined as

$$(2.24) \quad \varphi_m(x) = \begin{cases} \alpha \cdot x & \text{if } m = 0 \\ \alpha \cdot x^{m,0}(x) + \sum_{j=0}^{m-1} |x^{m,j+1}(x) - x^{m,j}(x)| & \text{if } m \geq 1 \end{cases}$$

for $x \in K_\sigma$, where the points

$$(2.25) \quad (x^{m,0}(x), \dots, x^{m,m}(x)) \in K_{\tau_0} \times \cdots \times K_{\tau_m}$$

satisfy

$$(2.26) \quad \begin{cases} x^{m,m}(x) = x \\ \alpha \cdot \nu(x^{m,0}(x)) < 0 \\ (x^{m,j+1}(x) - x^{m,j}(x)) \cdot \nu(x^{m,j}(x)) > 0, & 0 < j < m \\ \frac{x^{m,1}(x) - x^{m,0}(x)}{|x^{m,1}(x) - x^{m,0}(x)|} = \alpha - 2(\alpha \cdot \nu(x^{m,0}(x)))\nu(x^{m,0}(x)) \\ \frac{x^{m,j+1}(x) - x^{m,j}(x)}{|x^{m,j+1}(x) - x^{m,j}(x)|} = \frac{x^{m,j}(x) - x^{m,j-1}(x)}{|x^{m,j}(x) - x^{m,j-1}(x)|} \\ \quad - 2 \left(\frac{x^{m,j}(x) - x^{m,j-1}(x)}{|x^{m,j}(x) - x^{m,j-1}(x)|} \cdot \nu(x^{m,j}(x)) \right) \nu(x^{m,j}(x)), & 0 < j < m \end{cases}$$

and $\nu(x^{m,j}(x)) = \nu_{\tau_j}(x^{m,j}(x))$. Thus, using (2.24) in (2.16), the numerical approximation of each term in (2.23) can be effected following the single-scattering prescriptions described in Sect. 2.2.

2.4. Primitive periodic orbits and multiple scattering reformulation. While, as we mentioned, the formulation (2.22), (2.23) of the multiple-scattering effects can be used to reduce the problem of their numerical evaluation to that of solving a sequence of single-scattering problems, it is not the one that is best suited to analyze their asymptotic properties. To this end, it is more convenient to re-arrange the sum (2.22) in a manner that makes it explicit that the multiple-scattering contributions to the induced currents can be viewed as arising from a superposition of fields corresponding to *infinite, periodic* ray paths since, as we shall see, these are amenable to an analysis that can determine their asymptotic behavior.

The precise definition of these paths, which we shall refer to as “primitive periodic orbits”, is as follows:

Definition 2.2 (Primitive Periodic Orbits). For $n \geq 2$, we call an infinite sequence $\{\sigma_m\}_{m \geq 0} \in \mathcal{I}^{\mathbb{N}}$ a “primitive n -periodic orbit” if

$$\begin{aligned} \sigma_{n-1} &\neq \sigma_0 \\ \sigma_m &\neq \sigma_{m-1} \text{ for } m = 1, \dots, n-1 \\ \nexists m &\text{ with } l = \frac{n}{m} \in \mathbb{N} \text{ and } (\sigma_0, \dots, \sigma_{m-1})^l = (\sigma_0, \dots, \sigma_{n-1}) \\ \sigma_{m+jn} &= \sigma_m \text{ for } m = 0, \dots, n-1 \text{ and } j \geq 0; \end{aligned}$$

and denote by \mathcal{P}^n the collection of all primitive n -periodic orbits. For each $\sigma^n = \{\sigma_m^n\}_{m \geq 0} \in \mathcal{P}^n$, we define the corresponding “primitive n -periodic orbit correction”

$$\eta_{\sigma^n} = \{\eta_{\sigma_m^n}\}_{m \geq 0}$$

by

$$(2.27) \quad \eta_{\sigma_m^n} = \begin{cases} g_{\sigma_0^n} & \text{if } m = 0, \\ T_{\sigma_m^n \sigma_{m-1}^n} \eta_{\sigma_{m-1}^n} & \text{if } m > 0, \end{cases}$$

and we let

$$(2.28) \quad \bar{\eta}_{\sigma^n} = \{\bar{\eta}_{\sigma_m^n}\}_{m \geq n-1} = \{\eta_{\sigma_m^n}\}_{m \geq n-1}.$$

With this definition, the next result is now immediate.

Lemma 2.3 (Rearrangement into Primitive Periodic Orbits). *If the Neumann series (2.22) converges absolutely, then*

$$(2.29) \quad \eta = g + \sum_{n=2}^{\infty} \sum_{\sigma^n \in \mathcal{P}^n} \bar{\eta}_{\sigma^n}.$$

Note that explicitly, from (2.20) and (2.21), the components of $g = (g_{\sigma_1}, \dots, g_{\sigma_\tau})^t$ in (2.29) are the solutions of the integral equations

$$(2.30) \quad g_{\sigma}(x) - \int_{\partial K_{\sigma}} \frac{\partial G(x, y)}{\partial \nu(x)} g_{\sigma}(y) ds(y) = 2 \frac{\partial u^{\text{inc}}(x)}{\partial \nu(x)}, \quad x \in \partial K_{\sigma}$$

while the functions $\eta_{\sigma_m^n}$ in (2.28) that contribute to $\bar{\eta}_{\sigma^n}$ solve

$$(2.31) \quad \eta_{\sigma_m^n}(x) - \int_{\partial K_{\sigma_m^n}} \frac{\partial G(x, y)}{\partial \nu(x)} \eta_{\sigma_m^n}(y) ds(y) = \int_{\partial K_{\sigma_{m-1}^n}} \frac{\partial G(x, y)}{\partial \nu(x)} \eta_{\sigma_{m-1}^n}(y) ds(y), \quad x \in \partial K_{\sigma_m^n}.$$

Equivalently, the equations for the slow envelopes read

$$(2.32) \quad g_{\sigma}^{\text{slow}}(x) - \int_{\partial K_{\sigma}} \frac{\partial G(x, y)}{\partial \nu(x)} e^{ik(\varphi_0(y) - \varphi_0(x))} g_{\sigma}^{\text{slow}}(y) ds(y) = e^{-ik\varphi_0(x)} \left(2 \frac{\partial u^{\text{inc}}(x)}{\partial \nu(x)} \right), \quad x \in \partial K_{\sigma}$$

and

$$(2.33) \quad \eta_{\sigma_m^n}^{\text{slow}}(x) - \int_{\partial K_{\sigma_m^n}} \frac{\partial G(x, y)}{\partial \nu(x)} e^{ik(\varphi_{\sigma_m^n}(y) - \varphi_{\sigma_m^n}(x))} \eta_{\sigma_m^n}^{\text{slow}}(y) ds(y) \\ = e^{-ik\varphi_{\sigma_m^n}(x)} \int_{\partial K_{\sigma_{m-1}^n}} \frac{\partial G(x, y)}{\partial \nu(x)} e^{ik\varphi_{\sigma_{m-1}^n}(y)} \eta_{\sigma_{m-1}^n}^{\text{slow}}(y) ds(y),$$

for $x \in \partial K_{\sigma_m^n}$, where $\varphi_{\sigma_m^n}(x)$ is defined as in (2.24) on the path $(x^{m,0}(x), \dots, x^{m,m}(x)) \in K_{\sigma_0^n} \times \dots \times K_{\sigma_m^n}$ given by (2.26).

3. ASYMPTOTIC EXPANSIONS OF CURRENTS ON PERIODIC ORBITS

In this section we derive expressions for the asymptotic behavior of the currents $\eta_{\sigma_m^n}(x)$ in (2.31) with arbitrary period n . As we shall show in the following sections these formulas can be used to derive asymptotic convergence rates as the number of reflections increases and, moreover, they can also serve as the basis for acceleration strategies that allow for the attainment of accurate solutions with a reduced number of iterations.

For the derivations that follow we shall assume that the obstacles $\{K_\sigma : \sigma \in \mathcal{I}\}$ are *convex*, and that they satisfy

(a) the *visibility* condition

$$\forall \sigma, \tau, \rho \in \mathcal{I} : \overline{K_\rho} \cap \overline{\text{co}}(K_\sigma, K_\tau) \neq \emptyset \Rightarrow \rho \in \{\sigma, \tau\}$$

and

(b) the *no-occlusion* condition

$$\forall \sigma, \tau \in \mathcal{I} : \overline{\{x + t\alpha : x \in K_\sigma, t \in \mathbb{R}\}} \cap \overline{K_\tau} \neq \emptyset \Rightarrow \sigma = \tau.$$

These conditions guarantee that, for any given $x \in \partial K_{\sigma_m^n}$, the path $(x^{m,0}(x), \dots, x^{m,m}(x)) \in K_{\sigma_0^n} \times \dots \times K_{\sigma_m^n}$ determined by the conditions (2.26) is well-defined. For brevity, we shall henceforth refer to this path as the “broken $(m+1)$ -ray terminating at $x \in \partial K_{\sigma_m^n}$ ”. Further, the calculations below on the asymptotic behavior of the induced currents are independent of the periodicity of the path σ^n and we shall therefore simply write $K_m, \eta_m, x_m, t_m, \dots$, for $K_{\sigma_m^n}, \eta_{\sigma_m^n}, x_{\sigma_m^n}, t_{\sigma_m^n}, \dots$, to simplify the notation.

To state the main result in this section, we denote by

$$\Xi_p(x) \quad \text{and} \quad \kappa_p(x)$$

($p = 1, 2$) the unit vectors directed in principal directions and the principal curvatures, respectively, at $x \in \partial K$; and for $x \in \partial K_m$, we define $T_j^m(x), U_j^m(x), \kappa_j^m(x) \in \mathbb{R}^{2 \times 2}$, for $j = 0, \dots, m-1$, by setting

$$(T_j^m(x))_{pq} = F \left(\Xi_p(x^{m,j+1}(x)), \Xi_q(x^{m,j}(x)), \frac{x^{m,j+1}(x) - x^{m,j}(x)}{|x^{m,j+1}(x) - x^{m,j}(x)|} \right) \\ (U_j^m(x))_{pq} = F \left(\Xi_p(x^{m,j}(x)), \Xi_q(x^{m,j}(x)), \frac{x^{m,j+1}(x) - x^{m,j}(x)}{|x^{m,j+1}(x) - x^{m,j}(x)|} \right)$$

and

$$(\kappa_j^m(x))_{pq} = \kappa_p(x^{m,j}(x)) \delta_{pq}$$

where

$$(3.1) \quad F : S^2 \times S^2 \times S^2 \rightarrow \mathbb{R} : (u, v, w) \mapsto u \cdot v - u \cdot w v \cdot w$$

and δ_{pq} is the *Kronecker* delta. With this notation, the main result in this section is summarized in the following theorem.

Theorem 3.1. *For any $m \geq 0$, the iterated current η_m satisfies*

$$(3.2) \quad \eta_m^{\text{slow}}(x) = (1 + \mathcal{O}(k^{-1})) \begin{cases} 2ik \alpha \cdot \nu(x) & \text{if } m = 0 \\ \frac{x - x^{m,m-1}(x)}{|x - x^{m,m-1}(x)|} \cdot \nu(x) \frac{\eta_{m-1}^{\text{slow}}(x^{m,m-1}(x))}{\sqrt{\det N_m^m(x)}} & \text{if } m \geq 1 \end{cases}$$

as $k \rightarrow \infty$, on any compact subset of the illuminated region ∂K_m^{IL} . Here $N_j^m(x) \in \mathbb{R}^{2 \times 2}$ are defined by the recursion

$$(3.3) \quad N_1^m(x) = 2 [x^{m,1}(x) - x^{m,0}(x)] \cdot \nu(x^{m,0}(x)) \kappa_0^m(x) + U_0^m(x)$$

and, for $j = 2, \dots, m$,

$$\begin{aligned} N_j^m(x) &= 2 [x^{m,j}(x) - x^{m,j-1}(x)] \cdot \nu(x^{m,j-1}(x)) \kappa_{j-1}^m(x) + U_{j-1}^m(x) \\ &\quad + \frac{|x^{m,j}(x) - x^{m,j-1}(x)|}{|x^{m,j-1}(x) - x^{m,j-2}(x)|} \left(U_{j-1}^m(x) - T_{j-2}^m(x) [N_{j-1}^m(x)]^{-1} T_{j-2}^m(x)^t \right) \end{aligned}$$

In §4, our derivation of rate of convergence formulas on periodic orbits will be based on an analysis of the following version of Theorem 3.1 concerning the actual currents η_m .

Corollary 3.2. *For any $m \geq 1$, the iterated current η_m satisfies*

$$\eta_m(x) = (1 + \mathcal{O}(k^{-1})) 2ik \eta_m^A(x)$$

on any compact subset of ∂K_m^{IL} as $k \rightarrow \infty$. Here, η_m^A is defined over the whole boundary ∂K_m by

$$\eta_m^A(x) = (-1)^m e^{ik\varphi_m(x)} \beta_m(x) \gamma_m(x)$$

where

$$\beta_m(x) = \prod_{j=1}^m \frac{1}{\sqrt{\det N_j^m(x)}} \quad \text{and} \quad \gamma_m(x) = \prod_{j=0}^m \gamma_j^m(x);$$

$N_j^m(x)$ are as given in Theorem 3.1, and

$$\gamma_j^m(x) = \begin{cases} \frac{x^{m,j+1}(x) - x^{m,j}(x)}{|x^{m,j+1}(x) - x^{m,j}(x)|} \cdot \nu(x^{m,j}(x)) & \text{if } 0 \leq j \leq m-1 \\ \frac{x - x^{m,m-1}(x)}{|x - x^{m,m-1}(x)|} \cdot \nu(x) & \text{if } j = m \end{cases}$$

Proof. Given $x \in \partial K_m$, let (x^0, \dots, x^m) be the broken $(m+1)$ -ray terminating at x . As $\eta_m(x) = e^{ik\varphi_m(x)} \eta_m^{\text{slow}}(x)$, and

$$\alpha \cdot \nu(x^0) = -\gamma_0^m(x) \quad \text{and} \quad \frac{x^{j+1} - x^j}{|x^{j+1} - x^j|} \cdot \nu(x^j) = -\gamma_j^m(x)$$

($1 \leq j \leq m-1$), repeated application of Theorem 3.1 yields

$$\eta_m(x) = (1 + \mathcal{O}(k^{-1})) 2ik (-1)^m e^{ik\varphi_m(x)} \gamma_m(x) \prod_{j=1}^m \frac{1}{\sqrt{\det N_j^j(x^j)}}$$

Since, for $1 \leq j \leq m$, $N_j^m(x) = N_j^j(x^j)$, the result follows. \square

The proof of Theorem 3.1 is based on an asymptotic analysis of the integrals in (2.32)–(2.33). The first result below determines the asymptotic value of the right-hand side of (2.33), which correspond to the (normal derivative of) the field

$$(3.4) \quad u_{m-1}^{\text{scat}}(x) \equiv \int_{\partial K_{m-1}} G(x, y) \eta_{m-1}^{\text{slow}}(y) e^{ik\varphi_{m-1}(y)} ds(y) \quad x \in \mathbb{R}^2 \setminus \overline{K}_{m-1}$$

scattered by a current generated on the $m-1$ st obstacle in the path evaluated on the m th obstacle.

Lemma 3.3 (Asymptotic Expansions of Right-hand Sides). *For any $m \geq 1$, the asymptotic expansion, as $k \rightarrow \infty$, of the right-hand side of (2.33) coincides with the right-hand side of (3.2) on any compact subset of $\partial K_m \setminus \partial K_m^{SB}$.*

Proof. Given $x = x^m \in \partial K_m$, let $(x^0, \dots, x^m) \in \partial K_0 \times \dots \times \partial K_m$ be the broken $(m+1)$ -ray terminating at x . We write the right-hand side integral in (2.33) as

$$\int_{\partial K_{m-1}} \frac{\partial G(x, y)}{\partial \nu(x)} \eta_{m-1}^{\text{slow}}(y) e^{ik \varphi_{m-1}(y)} ds(y) = \sum_{j=1}^2 \int_{\partial K_{m-1}} \Lambda_j(y) \frac{\partial G(x, y)}{\partial \nu(x)} \eta_{m-1}^{\text{slow}}(y) e^{ik \varphi_{m-1}(y)} ds(y)$$

where Λ_1 and Λ_2 is a smooth partition of unity for the surface ∂K_{m-1} , and the support of Λ_1 is chosen to be a small neighborhood of x^{m-1} whose size is independent of k . Convexity, visibility and no-occlusion conditions combined with Lemma A.2 imply that [11] the integral involving Λ_2 is of order $\mathcal{O}(k^{-\infty})$ as $k \rightarrow \infty$. Concerning the integral involving $\Lambda_1(y)$, arguing exactly as in Lemma 3.4 in [6], and noting that $y = x^{m-1}$ is the only stationary point of the phase function $\Phi(x; y) = |x - y| + \varphi_{m-1}(y)$ in the support of Λ_1 , gives on account of the stationary phase lemma [9]

$$\begin{aligned} & \int_{\partial K_{m-1}} \Lambda_1(y) \frac{\partial G(x, y)}{\partial \nu(x)} \eta_{m-1}^{\text{slow}}(y) e^{ik \varphi_{m-1}(y)} ds(y) \\ &= \frac{1 - ik|x - x^{m-1}|}{k|x - x^{m-1}|^2} \frac{x - x^{m-1}}{|x - x^{m-1}|} \cdot \nu(x) \eta_{m-1}^{\text{slow}}(x^{m-1}) e^{ik\Phi(x; x^{m-1})} \frac{e^{i\pi[\text{sgn}(\text{Hess}[\Phi(x; x^{m-1})])]/4}}{\sqrt{|\det(\text{Hess}[\Phi(x; x^{m-1})])|}} \prod_{r=1}^2 |x_{t_r}^{m-1}| + \mathcal{O}(1) \end{aligned}$$

where sgn of a matrix is the number of positive eigenvalues minus the number of negative eigenvalues. The convexity assumption implies that $\text{sgn}(\text{Hess} \Phi(x; x^{m-1})) = 2$ since, in this case, all the eigenvalues of $\text{Hess} \Phi(x; x^{m-1})$ are necessarily expanding. Since

$$\det N_m^m(x) = |x - x^{m-1}|^2 \det(\text{Hess}[\Phi(x; x^{m-1})]) \prod_{r=1}^2 |x_{t_r}^{m-1}|^{-2}$$

we therefore obtain

$$\int_{\partial K_{m-1}} \Lambda_1(y) \frac{\partial G(x, y)}{\partial \nu(x)} \eta_{m-1}^{\text{slow}}(y) e^{ik \varphi_{m-1}(y)} ds(y) = \frac{x - x^{m-1}}{|x - x^{m-1}|} \cdot \nu(x) \frac{\eta_{m-1}^{\text{slow}}(x^{m-1})}{\sqrt{\det N_m^m(x)}} e^{ik\Phi(x; x^{m-1})} + \mathcal{O}(1)$$

and hence

$$\int_{\partial K_{m-1}} \frac{\partial G(x, y)}{\partial \nu(x)} \eta_{m-1}^{\text{slow}}(y) e^{ik \varphi_{m-1}(y)} ds(y) = \frac{x - x^{m-1}}{|x - x^{m-1}|} \cdot \nu(x) \frac{\eta_{m-1}^{\text{slow}}(x^{m-1})}{\sqrt{\det N_m^m(x)}} e^{ik\Phi(x; x^{m-1})} + \mathcal{O}(1)$$

Since the expression on the right-hand side of this expression is bounded away from zero, utilizing the identity $\varphi_m(x) = \Phi(x; x^{m-1})$ completes the proof. \square

Accordingly, to complete the proof of Theorem 3.1, we need to show that, for a target point in the m -th illuminated region, the corresponding left-hand side integral in (2.32)–(2.33) is negligible. This is the content of the next Lemma.

Lemma 3.4 (Asymptotic expansions of left-hand side integrals). *For any $m \geq 0$, we have*

$$(3.5) \quad \int_{\partial K_m} \frac{\partial G(x, y)}{\partial \nu(x)} e^{ik(\varphi_m(y) - \varphi_m(x))} \eta_m^{\text{slow}}(y) ds(y) = \mathcal{O}(k^{-1}) \eta_m^{\text{slow}}(x) + \mathcal{O}(k^{-1})$$

on any compact subset of ∂K_m^{IL} as $k \rightarrow \infty$.

Proof. Let S be a compact subset of ∂K_m^{IL} , and $x \in S$. As with the right-hand side integrals, we write

$$\int_{\partial K_m} \frac{\partial G(x, y)}{\partial \nu(x)} e^{ik(\varphi_m(y) - \varphi_m(x))} \eta_m^{\text{slow}}(y) ds(y) = \sum_{j=1}^2 \int_{\partial K_m} \Lambda_j(y) \frac{\partial G(x, y)}{\partial \nu(x)} e^{ik(\varphi_m(y) - \varphi_m(x))} \eta_m^{\text{slow}}(y) ds(y)$$

where Λ_1 and Λ_2 is a smooth partition of unity for the surface ∂K_{m-1} , but this time the support of Λ_1 is chosen to be a small (polar) neighborhood of x^m whose size is independent of k . Similar to the right-hand side integrals, the integral involving Λ_2 is of order $\mathcal{O}(k^{-\infty})$ as $k \rightarrow \infty$. To estimate the integral involving Λ_1 , let (t, τ) be the parametrization of the plane tangent to ∂K_m at the point x , and suppose that the surface ∂K_m is, locally, parametrized around x by $(t, \tau, f(t, \tau))$ so that $(0, 0, f(0, 0)) = (0, 0, 0)$ corresponds to x .

Therefore, setting $\Lambda(t, \tau) = \Lambda_1(y(t, \tau))$, $\varphi(t, \tau) = \varphi_m(y(t, \tau))$ and $\rho(t, \tau) = \eta_m^{\text{slow}}(y(t, \tau))$, the integral on the support of Λ_1 can be written in parametric form as

$$(3.6) \quad -\frac{1}{2\pi} \int_{\mathbb{R}^2} F(t, \tau) \rho(t, \tau) dt d\tau$$

where

$$F(t, \tau) = \Lambda(t, \tau) e^{ik\{d+\varphi(t,\tau)-\varphi(0,0)\}} \frac{ikd-1}{d^3} [f(t, \tau) - tf_t(0, 0) - \tau f_\tau(0, 0)] \sqrt{1 + f_t^2(t, \tau) + f_\tau^2(t, \tau)}$$

and $d = \sqrt{t^2 + \tau^2 + f^2(t, \tau)}$. To complete the proof, arguing as in the proof of Lemma 3.6 in [6], it suffices to show that

$$\int_{\mathbb{R}^2} F(t, \tau) dt d\tau = \mathcal{O}(k^{-1})$$

and, for a smooth function b vanishing at the origin,

$$\int_{\mathbb{R}^2} F(t, \tau) b(t, \tau) dt d\tau = \mathcal{O}(k^{-2}).$$

These equalities, on the other hand, follow from the invertability of the phase in F (cf. [12]), and the first order vanishing of F at the origin. \square

4. RATE OF CONVERGENCE ON PERIODIC ORBITS

Here we analyze the asymptotic expansions in Corollary 3.2 to derive high-frequency rate of convergence formulas for periodic orbits. Throughout this section, we shall suppose that $\{\sigma_m\}_{m \geq 0} \in \mathcal{I}^\infty$ is a fixed n -periodic multiple-scattering sequence (i.e. $\sigma_{m+1} \neq \sigma_m$ for all $m \geq 0$, and $\sigma_{r+qn} = \sigma_r$ for $0 \leq r \leq n-1$ and $q \geq 0$; as before, we will write K_m, η_m, \dots instead of $K_{\sigma_m}, \eta_{\sigma_m}, \dots$). As is apparent from Corollary 3.2, the analysis of the currents η_m on an n -periodic orbit requires the analysis of the ratios η_{m+n}^A/η_m^A and of the jointly illuminated regions $\partial K_{m+n}^{IL} \cap \partial K_m^{IL}$.

4.1. Properties of broken rays. In this section, we recall two classical results from the theory of dispersing billiard flows (see [6] and the references therein). The first one depends only on the convexity and the visibility conditions and is given in the next lemma.

Lemma 4.1. *There exist constants $C_1 = C_1(K)$ and $\delta_1 = \delta_1(K) < 1$ with the property that, given any sequence $\{\partial K_{\sigma_j}\}_{j=0, \dots, m}$ of obstacles with $\sigma_{j-1} \neq \sigma_j$ ($j = 1, \dots, m$), and any two sequences $\{\xi_j\}_{j=0, \dots, m}$ and $\{\zeta_j\}_{j=0, \dots, m}$ in $\partial K_{\sigma_0} \times \dots \times \partial K_{\sigma_m}$ satisfying the conditions*

- (a) *the segments $[\xi_{j-1}, \xi_j]$ and $[\xi_j, \xi_{j+1}]$ (resp. $[\zeta_{j-1}, \zeta_j]$ and $[\zeta_j, \zeta_{j+1}]$) satisfy the law of reflection at ξ_j (resp. ζ_j) ($j = 1, \dots, m-1$), and*
- (b) *neither of the segments $[\xi_{j-1}, \xi_j]$ or $[\zeta_{j-1}, \zeta_j]$ have a point in common with the interior of K ($j = 2, \dots, m-1$)*

we have

$$|\xi_j - \zeta_j| \leq C_1(\delta_1^j + \delta_1^{m-j}) \quad (0 \leq j \leq m).$$

In addition, we have

$$\xi_0 = \zeta_0 \quad \Rightarrow \quad |\xi_j - \zeta_j| \leq C_1 \delta_1^{m-j} \quad (0 \leq j \leq m),$$

and

$$\xi_m = \zeta_m \quad \Rightarrow \quad |\xi_j - \zeta_j| \leq C_1 \delta_1^j \quad (0 \leq j \leq m).$$

The second one, given in the next lemma, makes use of the no-occlusion condition in addition to convexity and visibility.

Lemma 4.2. *If $\alpha \in S^1 = \{\alpha \in \mathbb{R}^2 : |\alpha| = 1\}$ is such that the no-occlusion condition is satisfied, then there exist constants $C_2 = C_2(K, \alpha)$ and $\delta_2 = \delta_2(K, \alpha) < 1$ with the property that, for any two sequences $\{\xi_j\}_{j=0, \dots, m}$ and $\{\zeta_j\}_{j=0, \dots, m}$ satisfying the conditions in Lemma 4.1, the additional condition that these sequences correspond to broken rays with initial direction α implies*

$$|\xi_j - \zeta_j| \leq C_2 \delta_2^{m-j} \quad (0 \leq j \leq m).$$

4.2. Asymptotics of phase differences $\varphi_{m+n} - \varphi_m$ on n -periodic orbits. To characterize the asymptotic behavior of the phase differences $\varphi_{m+n} - \varphi_m$, we consider the “ n -periodic distance function”

$$(4.1) \quad \Phi_n(x^0, \dots, x^{n-1}) = |x^{n-1} - x^0| + \sum_{r=0}^{n-2} |x^{r+1} - x^r|$$

As the next lemma shows, the minimum of Φ_n has a very important geometric characterization.

Lemma 4.3. Φ_n attains its minimum at a uniquely determined point $(a^0, \dots, a^{n-1}) \in \partial K_0 \times \dots \times \partial K_{n-1}$. Moreover, with the extended definition

$$a^{r+qn} := a^r \quad \text{for} \quad [0 \leq r \leq n-1 \quad \text{and} \quad q \in \mathbb{Z}],$$

the points $\{a^j\}_{j \in \mathbb{Z}}$ satisfy

$$\frac{a^{j+1} - a^j}{|a^{j+1} - a^j|} = \frac{a^j - a^{j-1}}{|a^j - a^{j-1}|} - 2 \left(\frac{a^j - a^{j-1}}{|a^j - a^{j-1}|} \cdot \nu(a^j) \right) \nu(a^j).$$

That is, a ray starting from a^j and arriving at a^{j+1} transverses the path formed by the points $\{a^j\}_{j \in \mathbb{Z}}$ indefinitely.

Proof. Straightforward making use of convexity and visibility. \square

The next result depicts the relationship between the constant $\Phi_n(a^0, \dots, a^{n-1})$ and the phase differences $\varphi_{m+n} - \varphi_m$.

Lemma 4.4. For any $m > 2n$ and any $x \in \partial K_m$, we have

$$(4.2) \quad |\varphi_{m+n}(x) - \varphi_m(x) - \Phi_n(a^0, \dots, a^{n-1})| \leq C \delta^{m/2}$$

where the constants $C = C(K, \alpha)$ and $\delta = \delta(K, \alpha) \in (0, 1)$ are independent of the given periodic orbit.

Proof. Identical with its two dimensional version in [6]. \square

4.3. Asymptotics of the ratios β_{m+n}/β_m on n -periodic orbits. In this section, we derive explicit expressions for the limiting behavior of the ratios β_{m+n}/β_m on n -periodic orbits as $m \rightarrow \infty$. To this end, with $p = [m/2]$, we write

$$(4.3) \quad \frac{\beta_{m+n}(x)}{\beta_m(x)} = \left[\prod_{j=1}^{p-1} \frac{\det N_j^m(x)}{\det N_j^{m+n}(x)} \prod_{j=p}^m \frac{\det N_j^m(x)}{\det N_j^{m+n}(x)} \prod_{j=p}^{p+n-1} \frac{1}{\det N_j^{m+n}(x)} \right]^{1/2};$$

as we shall explain, the first two products on the right hand side of (4.3) can be approximated by 1, and the behavior of the last product is characterized by a sequence $\{N_j\}$, given in the next definition, determined by the geometry of the periodic orbit $\partial K_0 \times \dots \times \partial K_{n-1}$ at the points (a^0, \dots, a^{n-1}) .

Definition 4.5. The sequence $\{N_j\}_{j \geq 1} \subset \mathbb{R}^{2 \times 2}$ is defined by

$$(4.4) \quad N_1 = 2 [a^1 - a^0] \cdot \nu(a^0) \kappa_0 + U_0$$

and, for $j \geq 2$,

$$(4.5) \quad N_j = 2 [a^j - a^{j-1}] \cdot \nu(a^{j-1}) \kappa_{j-1} + U_{j-1} + \frac{|a^j - a^{j-1}|}{|a^{j-1} - a^{j-2}|} \left(U_{j-1} - T_{j-2} [N_{j-1}]^{-1} T_{j-2}^t \right)$$

where, utilizing the definition (3.1), $T_j, U_j, \kappa_j \in \mathbb{R}^{2 \times 2}$ are given by

$$(4.6) \quad (T_j)_{pq} = F \left(\Xi_p(a^{j+1}), \Xi_q(a^j), \frac{a^{j+1} - a^j}{|a^{j+1} - a^j|} \right) \quad [j \in \mathbb{Z}]$$

$$(4.7) \quad (U_j)_{pq} = F \left(\Xi_p(a^j), \Xi_q(a^j), \frac{a^{j+1} - a^j}{|a^{j+1} - a^j|} \right) \quad [j \in \mathbb{Z}]$$

and

$$(4.8) \quad (\kappa_j)_{pq} = \kappa_p(a^j) \delta_{pq} \quad [j \in \mathbb{Z}].$$

Remark 4.6. The matrices $N_m^m(x)$ and N_j are symmetric and positive definite. Indeed, for $m \geq 1$ and $x \in \partial K_m$, the matrix $N_m^m(x) \in \mathbb{R}^{2 \times 2}$ corresponds (through equations (A.8) and (A.9)) to the Hessian of the phase function Φ given by (A.1) at a point of (global) minimum of Φ , and is therefore symmetric and positive definite. This, in turn, implies through the identities $N_j^m(x) = N_j^j(x^{m,j}(x))$ ($1 \leq j \leq m$) that the matrices $N_j^m(x)$ are symmetric and positive definite. On the other hand, the matrices N_j ($j \geq 1$) correspond in a similar way to the Hessian (evaluated at a_{j-1}) of the phase function determined by a point source located at a_0 and has undergone j -bounces, and is therefore symmetric and positive definite.

The fact that the matrices $N_m^m(x)$ and N_j are symmetric and positive definite is essential since, in this case, their analysis is amenable to a treatment similar to their two dimensional versions in [6]. More precisely, using $\|\cdot\|$ to denote the operator norm, it can be readily verified that

$$(4.9) \quad |\det A| \leq (1 + \|A - I\|)^q$$

whenever $A \in \mathbb{R}^{q \times q}$. Accordingly, utilizing the identities

$$\frac{\det A}{\det B} = \det(AB^{-1}) = (\det(BA^{-1}))^{-1}$$

for invertible matrices, and using positive definiteness, we obtain

$$(4.10) \quad (1 + A_j^{m,n}(x))^{-1} \leq \left(\frac{\det N_j^m(x)}{\det N_j^{m+n}(x)} \right)^{1/2} \leq 1 + \mathcal{A}_j^{m,n}(x) \quad 1 \leq j < p$$

and

$$(4.11) \quad (1 + B_j^{m,n}(x))^{-1} \leq \left(\frac{\det N_j^m(x)}{\det N_{j+n}^{m+n}(x)} \right)^{1/2} \leq 1 + \mathcal{B}_j^{m,n}(x) \quad p \leq j < m$$

and

$$(4.12) \quad (1 + C_j^{m,n}(x))^{-1} \leq \left(\frac{\det N_{j-n}^m(x)}{\det N_j^{m+n}(x)} \right)^{1/2} \leq 1 + \mathcal{C}_j^{m,n}(x) \quad p \leq j < p+n$$

where we have set

$$(4.13) \quad \begin{aligned} A_j^{m,n}(x) &= \|N_j^{m+n}(x)N_j^m(x)^{-1} - I\|, & \mathcal{A}_j^{m,n}(x) &= \|N_j^m(x)N_j^{m+n}(x)^{-1} - I\| \quad [1 \leq j \leq p-1] \\ B_j^{m,n}(x) &= \|N_{j+n}^{m+n}(x)N_j^m(x)^{-1} - I\|, & \mathcal{B}_j^{m,n}(x) &= \|N_j^m(x)N_{j+n}^{m+n}(x)^{-1} - I\| \quad [p \leq j \leq m] \\ C_j^{m,n}(x) &= \|N_j^{m+n}(x)N_{j-n}^{-1} - I\|, & \mathcal{C}_j^{m,n}(x) &= \|N_{j-n}N_j^{m+n}(x)^{-1} - I\| \quad [p \leq j < p+n]. \end{aligned}$$

Utilizing the inequality

$$1 + x = e^x e^{\ln(1+x)-x} \leq e^x \quad \text{for } x \in [0, \infty],$$

we therefore obtain

$$(4.14) \quad \exp\left(-\sum_{j=1}^{p-1} A_j^{m,n}(x)\right) \leq \left(\prod_{j=1}^{p-1} \frac{\det N_j^m(x)}{\det N_j^{m+n}(x)}\right)^{1/2} \leq \exp\left(\sum_{j=1}^{p-1} \mathcal{A}_j^{m,n}(x)\right)$$

and

$$(4.15) \quad \exp\left(-\sum_{j=p}^m B_j^{m,n}(x)\right) \leq \left(\prod_{j=p}^m \frac{\det N_j^m(x)}{\det N_{j+n}^{m+n}(x)}\right)^{1/2} \leq \exp\left(\sum_{j=p}^m \mathcal{B}_j^{m,n}(x)\right)$$

and

$$(4.16) \quad \exp\left(-\sum_{j=p}^{p+n-1} C_j^{m,n}(x)\right) \leq \left(\prod_{j=p}^{p+n-1} \frac{\det N_{j-n}^m(x)}{\det N_j^{m+n}(x)}\right)^{1/2} \leq \exp\left(\sum_{j=p}^{p+n-1} \mathcal{C}_j^{m,n}(x)\right).$$

Comparing the expressions in (4.13) with their two dimensional versions in [6] (cf. Lemmas B.7 and B.8), it can be conjectured that

$$(4.17) \quad \begin{aligned} A_j^{m,n}(x) &\leq C\delta^{m-j} & \mathcal{A}_j^{m,n}(x) &\leq C\delta^{m-j} & [1 \leq j \leq p-1] \\ B_j^{m,n}(x) &\leq C\delta^j & \mathcal{B}_j^{m,n}(x) &\leq C\delta^j & [p \leq j \leq m] \\ C_j^{m,n}(x) &\leq C(\delta^{j-n} + \delta^{m-(j-n)}) & \mathcal{C}_j^{m,n}(x) &\leq C(\delta^{j-n} + \delta^{m-(j-n)}) & [p \leq j < p+n] \end{aligned}$$

for some constants C and $\delta \in (0, 1)$ depending only on K and α provided that $n < m/2$; we note that the only technicality in deriving (4.17) is the proof of equivalent versions of Lemmas B.2 and B.3 in [6] since then (4.17) follows exactly as in the proof of Lemmas B.7 and B.8 in [6] with only minor modifications; this technical analysis requires a study of the spectrum of the matrices $N_j^m(x)$ and will not be carried over in this paper. Inspired by the developments in [6], however, we shall assume that there exist constants $\vartheta = \vartheta(K, \alpha)$ and $\theta = \theta(K) > 1$ such that

$$(4.18) \quad \text{spec}(R_j^m(x)) \subset [\theta, \vartheta] \quad [1 \leq j \leq m], \quad \text{and} \quad \text{spec}(L_j) \subset [\theta, \vartheta] \quad [j \geq 1].$$

Following the same techniques in [6], and using (4.17) in (4.14), (4.15) and (4.16), one can then show that:

Lemma 4.7. *If (4.17) and (4.18) hold, then the limits*

$$(4.19) \quad \mathcal{N}_r = \lim_{q \rightarrow \infty} N_{r+qn} \quad [0 \leq r \leq n-1]$$

exist and, with the extended definition

$$(4.20) \quad \mathcal{N}_{r+qn} := \mathcal{N}_r \quad [0 \leq r \leq n-1 \quad \text{and} \quad q \in \mathbb{Z}],$$

they satisfy

$$(4.21) \quad \mathcal{N}_r = 2[a_r - a_{r-1}] \cdot \nu(a_{r-1}) \kappa_{r-1} + U_{r-1} + \frac{|a_r - a_{r-1}|}{|a_{r-1} - a_{r-2}|} \left(U_{r-1} - T_{r-2} [\mathcal{N}_{r-1}]^{-1} T_{r-2}^t \right) \quad [r \in \mathbb{Z}].$$

Moreover, for any $x \in \partial K_m$

$$\left| \frac{\beta_{m+n}(x)}{\beta_m(x)} - \prod_{r=0}^{n-1} \frac{1}{\sqrt{\det \mathcal{N}_r}} \right| \leq C \left(e^{C\delta^{m/2-n}} - 1 \right)$$

provided $n < m/2$ where the constants C and $\delta \in (0, 1)$ depend only on K and α , and are independent of the particular periodic orbit in consideration.

Closed form expressions for \mathcal{N}_r ($r = 0, \dots, n-1$) can be obtained based on equations (4.5), (4.19) and (4.20). In fact, these equations show that \mathcal{N}_0 determines $\{\mathcal{N}_r\}_{0 \leq r \leq n-1}$ uniquely through equation (4.21) which can also be used to obtain a (quadratic type matrix) equation for \mathcal{N}_0 .

For instance, when the period is $n = 2$, it can be readily verified that

$$U_0 = U_1 = I \quad \text{and} \quad T := T_0 = T_1^t$$

so that equation (4.21) gives

$$(4.22) \quad \mathcal{N}_0 = 2(I + d\kappa_1) - T[\mathcal{N}_1]^{-1}T^t$$

$$(4.23) \quad \mathcal{N}_1 = 2(I + d\kappa_0) - T^t[\mathcal{N}_0]^{-1}T.$$

Moreover, in this case, it is easy to show that T is a (real) unitary matrix. Therefore, multiplying (4.22) from the left by $T\mathcal{N}_1T^t$ yields

$$(4.24) \quad T\mathcal{N}_1T^t\mathcal{N}_0 = 2T\mathcal{N}_1T^t(I + d\kappa_1) - I;$$

on the other hand, multiplying (4.23) from the left by T and from the right by $T^t\mathcal{N}_0$ gives

$$(4.25) \quad T\mathcal{N}_1T^t\mathcal{N}_0 = 2T(I + d\kappa_0)T^t\mathcal{N}_0 - I.$$

Equations (4.24) and (4.25), in turn, yield

$$\mathcal{N}_1T^t(I + d\kappa_1) = (I + d\kappa_0)T^t\mathcal{N}_0$$

so that

$$(4.26) \quad \mathcal{N}_1 = (I + d\kappa_0) T^t \mathcal{N}_0 (I + d\kappa_1)^{-1} T$$

and

$$(4.27) \quad [\mathcal{N}_1]^{-1} = T^t (I + d\kappa_1) [\mathcal{N}_0]^{-1} T (I + d\kappa_0)^{-1} .$$

Using (4.27) in (4.22), we obtain

$$(4.28) \quad \mathcal{N}_0 = 2(I + d\kappa_1) - (I + d\kappa_1) [\mathcal{N}_0]^{-1} T (I + d\kappa_0)^{-1} T^t$$

so that multiplying (4.28) from the left by $(I + d\kappa_1)^{-1} \mathcal{N}_0 (I + d\kappa_1)^{-1}$ gives for

$$(4.29) \quad V = (I + d\kappa_1)^{-1} \mathcal{N}_0$$

the equation

$$V^2 - 2V + (I + d\kappa_1)^{-1} T (I + d\kappa_0)^{-1} T^t = 0 .$$

Formally, then

$$(4.30) \quad V = I \pm \sqrt{I - (I + d\kappa_1)^{-1} T (I + d\kappa_0)^{-1} T^t} .$$

Combining (4.26), (4.29) and (4.30), we therefore obtain

$$(4.31) \quad \mathcal{N}_0 \mathcal{N}_1 = (I + d\kappa_1) V (I + d\kappa_0) T^t (I + d\kappa_1) V (I + d\kappa_1)^{-1} T .$$

Since $\mathcal{N}_0 \mathcal{N}_1$ is positive definite, it can be readily verified through (4.31) that V must be taken with the plus sign in (4.30). Accordingly, combining (4.30) and (4.31), we obtain

$$\sqrt{\det(\mathcal{N}_0 \mathcal{N}_1)} = \sqrt{\det((I + d\kappa_0)(I + d\kappa_1))} \times \det \left(I + \sqrt{I - (I + d\kappa_1)^{-1} T (I + d\kappa_0)^{-1} T^t} \right) .$$

We note that this formula reduces to its two-dimensional version in [6] when scattering from two parallel infinite cylinders is considered.

4.4. Asymptotics of the differences $\gamma_{m+n} - \gamma_m$ on n -periodic orbits. To begin with, we note two simple geometrical facts.

Remark 4.8. The visibility condition holds if and only if there exists an angle $\phi_v \in (0, \pi/2)$ with the property that given any three points $\xi_1, \xi_2, \xi_3 \in \partial K$ such that the segments $[\xi_1, \xi_2]$ and $[\xi_2, \xi_3]$ (a) have no point in common with the interior of the connected component of K containing ξ_1 , and (b) satisfy the law of reflection at ξ_2 , we have

$$\frac{\xi_1 - \xi_2}{|\xi_1 - \xi_2|} \cdot \nu(\xi_2) = \frac{\xi_3 - \xi_2}{|\xi_3 - \xi_2|} \cdot \nu(\xi_2) \geq \cos \phi_v .$$

Similarly, the no-occlusion condition holds if and only if there exists an angle $\phi_{no} \in (0, \pi/2)$ with the property that given any two points $\xi_1, \xi_2 \in \partial K$ such that the segment $[\xi_1, \xi_2]$ have no point in common with the interior of the connected component of K containing ξ_1 , we have

$$\alpha \cdot \nu(\xi_1) = \frac{\xi_1 - \xi_2}{|\xi_1 - \xi_2|} \cdot \nu(\xi_1) \Rightarrow \frac{\xi_2 - \xi_1}{|\xi_2 - \xi_1|} \cdot \nu(\xi_1) \geq \cos \phi_{no} .$$

In what follows, we shall let $\phi_0 = \min\{\phi_v, \phi_{no}\}$.

We shall also make use of the following result.

Lemma 4.9 ([6]). *Let $\{A_j\}_{j \in S_A}$ and $\{B_j\}_{j \in S_B}$ be two sets of complex numbers. Then*

$$(4.32) \quad \left| \prod_{j \in S_A} A_j \prod_{j \in S_B} B_j - 1 \right| \leq \Upsilon \exp(\Upsilon)$$

where

$$\Upsilon = \sum_{j \in S_A} |A_j - 1| + \sum_{j \in S_B} |B_j - 1| .$$

Lemma 4.10. *There exist constants $C = C(K, \alpha)$ and $\delta = \delta(K, \alpha)$ such that, for any $m > 2n$ and $x \in \partial K_m$, we have*

$$|\gamma_{m+n}(x) - \gamma\gamma_m(x)| \leq C\delta^{(m-n)/2} \gamma \frac{\gamma_m(x)}{\gamma^{m,m}(x)} \leq C\delta^{(m-n)/2}$$

where

$$\gamma = \prod_{j=0}^{n-1} \gamma^j$$

and

$$\gamma^j = \frac{a^{j+1} - a^j}{|a^{j+1} - a^j|} \cdot \nu(a^j) \quad \text{for } j \in \mathbb{Z}.$$

Proof. For $0 \leq j \leq m-1$, we have

$$\begin{aligned} \gamma^{m+n,j}(x) - \gamma^{m,j}(x) &= \frac{x^{m,j+1}(x) - x^{m,j}(x)}{|x^{m,j+1}(x) - x^{m,j}(x)|} \cdot (\nu(x^{m+n,j}(x)) - \nu(x^{m,j}(x))) \\ &+ \frac{|x^{m,j+1}(x) - x^{m,j}(x)| - |x^{m+n,j+1}(x) - x^{m+n,j}(x)|}{|x^{m,j+1}(x) - x^{m,j}(x)|} \gamma_j^{m+n}(x) \\ &+ \frac{x^{m+n,j+1}(x) - x^{m,j+1}(x) + x^{m,j}(x) - x^{m+n,j}(x)}{|x^{m,j+1}(x) - x^{m,j}(x)|} \cdot \nu(x^{m+n,j}(x)) \end{aligned}$$

so that

$$\begin{aligned} |\gamma^{m+n,j}(x) - \gamma^{m,j}(x)| &\leq |\nu(x^{m+n,j}(x)) - \nu(x^{m,j}(x))| \\ &+ \frac{2}{d_{\min}} (|x^{m+n,j+1}(x) - x^{m,j+1}(x)| + |x^{m+n,j}(x) - x^{m,j}(x)|); \end{aligned}$$

therefore

$$C^{-1} |\gamma^{m+n,j}(x) - \gamma^{m,j}(x)| \leq |x^{m+n,j+1}(x) - x^{m,j+1}(x)| + |x^{m+n,j}(x) - x^{m,j}(x)|$$

for some constant $C = C(K)$. Accordingly, by Lemma 4.2, we obtain

$$|\gamma^{m+n,j}(x) - \gamma^{m,j}(x)| \leq CC_2(\delta^{m-(j+1)} + \delta^{m-j}) = CC_2(1 + \delta)\delta^{m-(j+1)}$$

for $0 \leq j \leq m-1$. Following the same steps, and applying Lemma 4.1, we get

$$|\gamma^{m+n,j+n}(x) - \gamma^{m,j}(x)| \leq CC_1(1 + \delta)\delta^j \quad [0 \leq j \leq m];$$

and by a similarly procedure and using Lemmas 4.1 and 4.3, we obtain

$$|\gamma^{m+n,j}(x) - \gamma^j| \leq CC_1(1 + \delta)(\delta^{m-(j+1)} + \delta^j) \quad [0 \leq j \leq m-1].$$

Now, choosing $p = [(m-n)/2]$

$$A_j = \begin{cases} \frac{\gamma^{m+n,j}(x)}{\gamma^{m,j}(x)} & \text{for } 0 \leq j \leq p-1 \\ \frac{\gamma^{m+n,j+n}(x)}{\gamma^{m,j}(x)} & \text{for } p \leq j \leq m-1 \end{cases}$$

and

$$B_j = \frac{\gamma^{m+n,j}(x)}{\gamma^j} \quad \text{for } p \leq j \leq p+n-1$$

we therefore obtain by Lemma 4.9 and Remark 4.8

$$\left| \frac{\prod_{j=0}^{m+n-1} \gamma^{m+n,j}(x)}{\gamma \prod_{j=0}^{m-1} \gamma^{m,j}(x)} - 1 \right| \leq \Upsilon \exp(\Upsilon)$$

where, with $C_3 = C(1 + \delta) \max\{C_1, C_2\} / \cos(\phi_0)$,

$$C_3^{-1} \Upsilon = \sum_{j=0}^{p-1} \delta^{m-(j+1)} + \sum_{j=p}^{m-1} \delta^j + \sum_{j=p}^{p+n-1} (\delta^{m-(j+1)} + \delta^j).$$

Since

$$(1 - \delta)C_3^{-1}\Upsilon \leq \delta^{m-p} + \delta^p + \delta^{m-(p+n)} + \delta^p \leq 2(\delta^p + \delta^{m-(p+n)}) \leq 4\delta^p,$$

we therefore get, with $C_4 = 4(1/\delta - 1)C_3 \exp(4(1/\delta - 1)C_3)$,

$$\left| \prod_{j=0}^{m+n-1} \gamma^{m+n,j}(x) - \gamma \prod_{j=0}^{m-1} \gamma^{m,j}(x) \right| \leq C_4 \delta^{(m-n)/2} \gamma \prod_{j=0}^{m-1} \gamma^{m,j}(x).$$

Equivalently

$$\left| \frac{\gamma_{m+n}(x)}{\gamma^{m+n,m+n}(x)} - \gamma \frac{\gamma_m(x)}{\gamma^{m,m}(x)} \right| \leq C_4 \delta^{(m-n)/2} \gamma \frac{\gamma_m(x)}{\gamma^{m,m}(x)}.$$

Now, with $j_1 = m - 1$ and $j_2 = m + n - 1$, we have

$$\begin{aligned} \gamma^{m+n,m+n}(x) - \gamma^{m,m}(x) &= \frac{x^{m,j_1}(x) - x^{m+n,j_2}(x)}{|x - x^{m,j_1}(x)|} \cdot \nu(x) \\ &+ \frac{|x - x^{m,j_1}(x)| - |x - x^{m+n,j_2}(x)|}{|x - x^{m,j_1}(x)|} \frac{x - x^{m+n,j_2}(x)}{|x - x^{m+n,j_2}(x)|} \cdot \nu(x) \end{aligned}$$

so that

$$|\gamma^{m+n,m+n}(x) - \gamma^{m,m}(x)| \leq \frac{2}{d_{\min}} |x^{m+n,j_2}(x) - x^{m,j_1}(x)| \leq C_5 \delta^m$$

where we have applied Lemma 4.1, and set $C_5 = 2C_1/(\delta d_{\min})$. Since

$$\gamma_{m+n}(x) - \gamma \gamma_m(x) = (\gamma^{m+n,m+n}(x) - \gamma^{m,m}(x)) \gamma \frac{\gamma_m(x)}{\gamma^{m,m}(x)} + \gamma^{m+n,m+n}(x) \left(\frac{\gamma_{m+n}(x)}{\gamma^{m+n,m+n}(x)} - \gamma \frac{\gamma_m(x)}{\gamma^{m,m}(x)} \right)$$

we therefore obtain the result with $C = 2 \max\{C_4, C_5\}$. \square

4.5. Rate of convergence formulas on n -periodic orbits. In this section, we combine the above analysis concerning the asymptotic behaviors of iterated currents *only* on the jointly illuminated regions, to derive high-frequency rate of convergence formulas on periodic orbits that are valid not only on the jointly illuminated regions but over the *entire* surfaces ∂K_m . To this end, first we state our main result concerning the asymptotic behavior of the approximate currents η_m that follows from a combination of Lemmas 4.4, 4.7 and 4.10 utilizing the techniques in [6].

Theorem 4.11. *Provided that conditions (4.17) and (4.18) hold, the n -periodic limits*

$$\mathcal{N}_r = \lim_{q \rightarrow \infty} N_{r+qn} \quad [0 \leq r \leq n-1]$$

of the sequence $\{N_j\}_{j \geq 1}$ introduced in Definition 4.5 exist and

$$\text{spec}(\mathcal{N}_r) \subset [\theta, \vartheta] \quad [0 \leq r \leq n-1]$$

where ϑ and $\theta > 1$ are as in (4.18); with the extended definition

$$\mathcal{N}_{r+qn} := \mathcal{N}_r \quad [0 \leq r \leq n-1 \quad \text{and} \quad q \in \mathbb{Z}],$$

they satisfy the recursion

$$\mathcal{N}_r = 2[a_r - a_{r-1}] \cdot \nu(a_{r-1}) \kappa_{r-1} + U_{r-1} + \frac{|a_r - a_{r-1}|}{|a_{r-1} - a_{r-2}|} \left(U_{r-1} - T_{r-2} [\mathcal{N}_{r-1}]^{-1} T_{r-2}^t \right) \quad [r \in \mathbb{Z}].$$

Moreover, for any $m > 2n$ and $x \in \partial K_m$, we have

$$\left| \eta_{m+n}^A(x) - \mathcal{R}_{n,k} \eta_m^A(x) \right| \leq \left| \frac{\eta_m^A(x)}{\gamma^{m,m}(x)} \right| \mathcal{F} \leq \delta^{m/2} \mathcal{F}$$

where

$$\mathcal{R}_{n,k} = (-1)^n e^{ik\Phi_n(a^0, \dots, a^{n-1})} \prod_{r=0}^{n-1} \frac{1}{\sqrt{\det \mathcal{N}_r}} \prod_{r=0}^{n-1} \frac{a^{r+1} - a^r}{|a^{r+1} - a^r|} \cdot \nu(a^r),$$

$$\mathcal{F} = \mathcal{F}(C, k, \delta, m, n) = \min \left\{ 2, e^{Ck\delta^{m/2}} - 1 \right\} \delta^{n/2} + C \left[\delta^{(m-n)/2} + \left(e^{C\delta^{m/2-n}} - 1 \right) \right]^2$$

and the constants $C = C(K, \alpha)$ and $\delta = \delta(K, \alpha) \in (0, 1)$ are independent of the given periodic orbit.

Remark 4.12. It is important to note that the dependency of the rate of convergence formulas (namely $\mathcal{R}_{n,k}$) on the relative rotations of the structures are embedded within the matrices \mathcal{N}_r . For instance, this is clearly visible from the two-periodic rate of convergence formulas

$$(4.33) \quad \mathcal{R}_{2,k} = e^{2ikd} \left(\sqrt{\det [(I + d\kappa_1)(I + d\kappa_2)]} \times \det \left[I + \sqrt{I - [T(I + d\kappa_1)T^{-1}(I + d\kappa_2)]^{-1}} \right] \right)^{-1}$$

where $d = \text{dist}(K_1, K_2) = |a_1 - a_2|$ is the distance, κ_i are the matrices of *principal curvatures* at the points a_i , and T is a unitary matrix that depends on the *rotation* between the principal axis at these points.

Next we present a purely geometric result that guarantees the existence of *fixed* compact subsets T_r and S_r of ∂K_r ($r = 0, \dots, n-1$) with the property that, for all sufficiently large m ,

$$T_r \subset\subset S_r \subset \partial K_{m+n}^{IL} \cap \partial K_m^{IL} \quad \text{provided } m \equiv r \pmod{n}$$

and the obstacle K_{m+1} falls into the region spanned by the rays reflecting from T_r at the m and $(m+n)$ -th reflections. The proof, being essentially the same as that of Theorem 4.2 in [6], is omitted.

Theorem 4.13. *For $0 \leq r \leq n-1$, there exist compact connected subsets S_r and T_r of ∂K_r with the property that*

$$\exists m_0 \geq 1 : \forall m \geq m_0 \quad [m \equiv r \pmod{n}] \Rightarrow J_{m+1}(\partial K_{m+1}) \subset T_r \subset \text{int}(S_r) \subset S_r \subset \partial K_m^{IL}$$

where, for $m \geq 1$, $J_m : \partial K_m \rightarrow \partial K_{m-1} : x \mapsto x_{m-1}^m(x)$.

Finally, we combine Theorems 4.11 and 4.13 to obtain high-frequency rate of convergence formulas. Indeed, appealing to Corollary 3.2, we have

$$\eta_m(x) = (1 + k^{-1}P_m(x, k)) 2ik \eta_m^A(x) \quad \text{as } k \rightarrow \infty$$

on any compact subset of ∂K_m^{IL} where $P_m(k, x) = \mathcal{O}(k^0)$. Accordingly

$$\begin{aligned} \eta_{m+n}(x) - \mathcal{R}_{n,k} \eta_m(x) &= \frac{P_{m+n}(x, k) - P_m(x, k)}{k + P_m(x, k)} \mathcal{R}_{n,k} \eta_m(x) \\ &\quad + \frac{k + P_{m+n}(x, k)}{k + P_m(x, k)} 2ik \left(1 + \frac{P_m(x, k)}{k} \right) (\eta_{m+n}^A(x) - \mathcal{R}_{n,k} \eta_m^A(x)) \end{aligned}$$

holds, as $k \rightarrow \infty$, on any compact subset of the jointly illuminated regions $\partial K_{m+n}^{IL} \cap \partial K_m^{IL}$; Theorem 4.11, in turn, yields

$$\begin{aligned} |\eta_{m+n}(x) - \mathcal{R}_{n,k} \eta_m(x)| &\leq \left| \frac{P_{m+n}(x, k) - P_m(x, k)}{k + P_m(x, k)} \right| |\mathcal{R}_{n,k}| |\eta_m(x)| \\ &\quad + \left| \frac{k + P_{m+n}(x, k)}{k + P_m(x, k)} \right| \left| 2ik \left(1 + \frac{P_m(x, k)}{k} \right) \eta_m^A(x) \right| \left| \frac{\mathcal{F}}{\gamma^{m,m}(x)} \right| \end{aligned}$$

so that, since $|\gamma^{m,m}(x)| \leq 1$, we get

$$\begin{aligned} |\eta_{m+n}(x) - \mathcal{R}_{n,k} \eta_m(x)| &\leq \left(\left| \frac{P_{m+n}(x, k) - P_m(x, k)}{k + P_m(x, k)} \right| |\mathcal{R}_{n,k}| + \left| \frac{k + P_{m+n}(x, k)}{k + P_m(x, k)} \right| |\mathcal{F}| \right) \left| \frac{\eta_m(x)}{\gamma^{m,m}(x)} \right| \\ &:= (\mathcal{S}_{m,n}(x, k) |\mathcal{R}_{n,k}| + \mathcal{T}_{m,n}(x, k) |\mathcal{F}|) \left| \frac{\eta_m(x)}{\gamma^{m,m}(x)} \right| \end{aligned}$$

on any compact subset of $\partial K_{m+n}^{IL} \cap \partial K_m^{IL}$ as $k \rightarrow \infty$. As $|\mathcal{R}_{n,k}| \leq \delta^{n/2}$, and $|\gamma^{m,m}|$ is bounded away from zero on any compact subset of ∂K_m^{IL} , replacing δ in Theorem 4.11 with $\delta^{1/2}$, we obtain the following result.

Corollary 4.14. *Under the assumptions of Theorem 4.11, on any compact subset of the jointly illuminated regions $\partial K_{m+n}^{IL} \cap \partial K_m^{IL}$, if $\mathcal{S}_{m,n}(x, k) = \mathcal{O}(k^{-1})$ and $\mathcal{T}_{m,n}(x, k) = \mathcal{O}(k^0)$ as $k \rightarrow \infty$ independently of m , then*

$$(4.34) \quad \begin{aligned} |\eta_{m+n}(x) - \mathcal{R}_{n,k} \eta_m(x)| &= (\mathcal{O}(k^{-1} \delta^n) + \mathcal{O}(k^0 \mathcal{F})) |\eta_m(x)| \\ &= (\mathcal{O}(k^{-1} \delta^n) + \mathcal{O}(k \delta^{m+n}) + \mathcal{O}(k^0 \delta^{m-2n})) |\eta_m(x)| \end{aligned}$$

provided $m > 2n$ where all the order terms depend only on the compact subset in consideration.

We finally note that, as we have shown in [6], Theorem 4.13 ensures the validity of rate of convergence formulas implied by the approximation (4.34) over the *entire* boundaries ∂K_m .

5. NUMERICAL RESULTS

In this section, we present numerical examples testing our rate of convergence formula

$$(5.1) \quad \left\| \frac{\eta_{m+n}(x)}{\eta_m(x)} - \mathcal{R}_{n,k} \right\|_{L_\infty(\partial K_m)} = \mathcal{O}(k^{-1}\delta^n) + \mathcal{O}(k\delta^{m+n}) + \mathcal{O}(k^0\delta^{m-2n}),$$

that follows from (4.34), on two-periodic orbits. As is apparent from (5.1), for a two-periodic orbit, one should observe the following numerical behavior:

$$(5.2) \quad \left\| \frac{\eta_{m+2}(x)}{\eta_m(x)} - \mathcal{R}_{2,k} \right\|_{L_\infty(\partial K_m)} = \mathcal{O}(k^{-1}) + \mathcal{O}(k\delta^m).$$

As a first step in testing the validity of (5.2), in Tables 1–2, we display a comparison of

$$(5.3) \quad \frac{\|\eta_{m+2}\|_{L_\infty}}{\|\eta_m\|_{L_\infty}}$$

and $|\mathcal{R}_{2,k}|$ for a variety of configurations. Specifically, Table 1 depicts this comparison for two different configurations; Table 2, on the other hand, displays the dependencies with respect to rotation. As is apparent from these Tables, $|\mathcal{R}_{2,k}|$ provides a good approximation to (5.3), and in fact, the quality of the approximation improves with increasing frequency.

As we anticipated, a distinctive property of our three-dimensional rate of convergence formulas (compared to their two-dimensional counterparts in [6]) is that in three-dimensional configurations these formulas depend on the relative rotation of principal axis at the points (a^0, \dots, a^{n-1}) . We have therefore displayed

$$(5.4) \quad \left\| \frac{\eta_{m+2}(x)}{\eta_m(x)} - \mathcal{R}_{2,k} \right\|_{L_\infty(\partial K_m)}$$

for the two ellipsoids

$$(5.5) \quad S_1 : \frac{x^2}{1^2} + \frac{(y+1/4)^2}{(1/2)^2} + \frac{z^2}{(1/2)^2} = 1 \quad \text{and} \quad S_2 : \frac{x^2}{1^2} + \frac{(y-1)^2}{(1/2)^2} + \frac{z^2}{(1/2)^2} = 1$$

in Table 3. More specifically, Table 3 depicts (5.4) for the rotations of S_2 by $0, \pi/6, \pi/4, \pi/3$ and $\pi/2$ with respect to the y -axis (in the counter-clockwise direction) keeping the ellipsoid S_1 fixed. As is apparent from Table 3, our rate of convergence formula (5.4) provides a good approximation, whose accuracy increases with increasing frequency, for the convergence of multiple scattering iterates on periodic orbits. Moreover, as implied by our formulas, this table shows that the rate does not depend on the particular direction of incidence.

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$$K_0 = S_1 \quad \|\eta_{2m}\|/\|\eta_{2m-2}\| \qquad K_0 = S_1 \quad \|\eta_{2m+1}\|/\|\eta_{2m-1}\|$$

m	k = 4	k = 8	k = 16	k = 32	m	k = 4	k = 8	k = 16	k = 32
1	0.1043	0.0886	0.0814	0.0782	1	0.0846	0.0789	0.0766	0.0758
2	0.0793	0.0747	0.0729	0.0724	2	0.0785	0.0741	0.0741	0.0720
3	0.0785	0.0740	0.0724	0.0720	3	0.0785	0.0740	0.0724	0.0720
4	0.0785	0.0740	0.0724	0.0720	4	0.0785	0.0740	0.0724	0.0720
5	0.0785	0.0740	0.0724	0.0720	5	0.0785	0.0740	0.0724	0.0720

$$K_0 = S_2 \quad \|\eta_{2m}\|/\|\eta_{2m-2}\| \qquad K_0 = S_2 \quad \|\eta_{2m+1}\|/\|\eta_{2m-1}\|$$

m	k = 4	k = 8	k = 16	k = 32	m	k = 4	k = 8	k = 16	k = 32
1	0.1043	0.0886	0.0814	0.0782	1	0.0846	0.0789	0.0766	0.0758
2	0.0793	0.0748	0.0729	0.0724	2	0.0785	0.0741	0.0741	0.0720
3	0.0785	0.0740	0.0724	0.0720	3	0.0785	0.0740	0.0724	0.0720
4	0.0785	0.0740	0.0724	0.0720	4	0.0785	0.0740	0.0724	0.0720
5	0.0785	0.0740	0.0724	0.0720	5	0.0785	0.0740	0.0724	0.0720

Two unit spheres S_1 and S_2 with centers $C_1 = (-\frac{3}{2}, 0, 0)$ and $C_2 = (\frac{3}{2}, 0, 0)$;
 $\alpha = (0, 0, -1)$ and $|\mathcal{R}_{2,k}| \approx 0.0718$.

$$K_0 = S_1 \quad \|\eta_{2m}\|/\|\eta_{2m-2}\| \qquad K_0 = S_1 \quad \|\eta_{2m+1}\|/\|\eta_{2m-1}\|$$

m	k = 4	k = 8	k = 16	k = 32	k=64	m	k = 4	k = 8	k = 16	k = 32	k=64
1	0.3867	0.2625	0.2041	0.1754	0.1632	1	0.2071	0.1719	0.1506	0.1400	0.1353
2	0.1730	0.1488	0.1334	0.1268	0.1245	2	0.1664	0.1440	0.1308	0.1246	0.1226
3	0.1652	0.1431	0.1300	0.1242	0.1222	3	0.1651	0.1430	0.1299	0.1241	0.1222
4	0.1651	0.1430	0.1299	0.1241	0.1221	4	0.1651	0.1430	0.1299	0.1241	0.1221
5	0.1651	0.1430	0.1299	0.1241	0.1221	5	0.1651	0.1430	0.1299	0.1241	0.1221
6	0.1651	0.1430	0.1299	0.1241	0.1221	6	0.1651	0.1430	0.1299	0.1241	0.1221
7	0.1651	0.1430	0.1299	0.1241	0.1221	7	0.1651	0.1430	0.1299	0.1241	0.1221
8	0.1651	0.1430	0.1299	0.1241	0.1221	8	0.1651	0.1430	0.1299	0.1241	0.1221

$$K_0 = S_2 \quad \|\eta_{2m}\|/\|\eta_{2m-2}\| \qquad K_0 = S_2 \quad \|\eta_{2m+1}\|/\|\eta_{2m-1}\|$$

m	k = 4	k = 8	k = 16	k = 32	k=64	m	k = 4	k = 8	k = 16	k = 32	k=64
1	0.3174	0.2227	0.1791	0.1560	0.1459	1	0.2048	0.1678	0.1488	0.1389	0.1347
2	0.1724	0.1487	0.1337	0.1270	0.1247	2	0.1661	0.1437	0.1306	0.1245	0.1225
3	0.1652	0.1431	0.1300	0.1232	0.1222	3	0.1651	0.1430	0.1299	0.1241	0.1221
4	0.1651	0.1430	0.1299	0.1241	0.1221	4	0.1651	0.1430	0.1299	0.1241	0.1221
5	0.1651	0.1430	0.1299	0.1241	0.1221	5	0.1651	0.1430	0.1299	0.1241	0.1221
6	0.1651	0.1430	0.1299	0.1241	0.1221	6	0.1651	0.1430	0.1299	0.1241	0.1221
7	0.1651	0.1430	0.1299	0.1241	0.1221	7	0.1651	0.1430	0.1299	0.1241	0.1221
8	0.1651	0.1430	0.1299	0.1241	0.1221	8	0.1651	0.1430	0.1299	0.1241	0.1221

Two ellipsoids S_1 and S_2 with radii $R_1 = (1/2, 1, 1/2)$, $R_2 = (1, 1/2, 1/2)$
and centers $C_1 = (0, -3/4, 0)$, $C_2 = (0, 1, 0)$; $\alpha = (0, 0, -1)$ and $|\mathcal{R}_{2,k}| \approx 0.1214$.

TABLE 1. Comparison of (5.3) and $|\mathcal{R}_{2,k}|$ for two different configurations.

$K_0 = S_1 \quad \ \eta_{2m}\ /\ \eta_{2m-2}\ $						$K_0 = S_1 \quad \ \eta_{2m+1}\ /\ \eta_{2m-1}\ $					
m	k = 4	k = 8	k = 16	k = 32	k=64	m	k = 4	k = 8	k = 16	k = 32	k=64
1	0.4251	0.3393	0.2922	0.2665	0.2542	1	0.3353	0.2992	0.2819	0.2724	0.2682
2	0.2918	0.2665	0.2548	0.2502	0.2488	2	0.2754	0.2551	0.2443	0.2404	0.2393
3	0.2691	0.2499	0.2403	0.2366	0.2357	3	0.2669	0.2481	0.2387	0.2351	0.2343
4	0.2661	0.2475	0.2381	0.2346	0.2337	4	0.2658	0.2472	0.2378	0.2344	0.2336
5	0.2657	0.2472	0.2378	0.2343	0.2335	5	0.2657	0.2471	0.2377	0.2343	0.2335
6	0.2657	0.2471	0.2377	0.2343	0.2335	6	0.2657	0.2471	0.2377	0.2343	0.2335
7	0.2657	0.2471	0.2377	0.2343	0.2335	7	0.2657	0.2471	0.2377	0.2343	0.2335
8	0.2657	0.2471	0.2377	0.2343	0.2335	8	0.2657	0.2471	0.2377	0.2343	0.2335

$K_0 = S_2 \quad \ \eta_{2m}\ /\ \eta_{2m-2}\ $						$K_0 = S_2 \quad \ \eta_{2m+1}\ /\ \eta_{2m-1}\ $					
m	k = 4	k = 8	k = 16	k = 32	k=64	m	k = 4	k = 8	k = 16	k = 32	k=64
1	0.4251	0.3393	0.2922	0.2665	0.2542	1	0.3353	0.2992	0.2819	0.2724	0.2682
2	0.2918	0.2665	0.2548	0.2502	0.2488	2	0.2754	0.2551	0.2443	0.2404	0.2393
3	0.2691	0.2499	0.2403	0.2366	0.2357	3	0.2669	0.2481	0.2387	0.2351	0.2343
4	0.2661	0.2475	0.2381	0.2346	0.2337	4	0.2658	0.2472	0.2378	0.2344	0.2336
5	0.2657	0.2472	0.2378	0.2343	0.2335	5	0.2657	0.2471	0.2377	0.2343	0.2335
6	0.2657	0.2471	0.2377	0.2343	0.2335	6	0.2657	0.2471	0.2377	0.2343	0.2335
7	0.2657	0.2471	0.2377	0.2343	0.2335	7	0.2657	0.2471	0.2377	0.2343	0.2335
8	0.2657	0.2471	0.2377	0.2343	0.2335	8	0.2657	0.2471	0.2377	0.2343	0.2335

$$\theta = 0$$

$$|\mathcal{R}_{2,k}| \approx 0.2329$$

$K_0 = S_1 \quad \ \eta_{2m}\ /\ \eta_{2m-2}\ $						$K_0 = S_1 \quad \ \eta_{2m+1}\ /\ \eta_{2m-1}\ $					
m	k = 4	k = 8	k = 16	k = 32	k=64	m	k = 4	k = 8	k = 16	k = 32	k=64
1	0.2945	0.2570	0.2287	0.2087	0.1970	1	0.3139	0.2748	0.2585	0.2488	0.2445
2	0.2777	0.2533	0.2417	0.2378	0.2357	2	0.2568	0.2387	0.2281	0.2245	0.2234
3	0.2536	0.2357	0.2270	0.2232	0.2221	3	0.2521	0.2343	0.2255	0.2223	0.2213
4	0.2519	0.2341	0.2253	0.2222	0.2211	4	0.2518	0.2340	0.2252	0.2221	0.2210
5	0.2518	0.2340	0.2252	0.2221	0.2210	5	0.2518	0.2340	0.2252	0.2220	0.2210
6	0.2518	0.2340	0.2252	0.2220	0.2210	6	0.2518	0.2340	0.2252	0.2220	0.2210
7	0.2518	0.2340	0.2252	0.2220	0.2210	7	0.2518	0.2340	0.2252	0.2220	0.2210
8	0.2518	0.2340	0.2252	0.2220	0.2210	8	0.2518	0.2340	0.2252	0.2220	0.2210

$K_0 = S_2 \quad \ \eta_{2m}\ /\ \eta_{2m-2}\ $						$K_0 = S_2 \quad \ \eta_{2m+1}\ /\ \eta_{2m-1}\ $					
m	k = 4	k = 8	k = 16	k = 32	k=64	m	k = 4	k = 8	k = 16	k = 32	k=64
1	0.4100	0.3204	0.2778	0.2562	0.2467	1	0.3307	0.2994	0.2864	0.2776	0.2725
2	0.2672	0.2454	0.2358	0.2313	0.2296	2	0.2587	0.2498	0.2302	0.2266	0.2252
3	0.2530	0.2352	0.2261	0.2228	0.2217	3	0.2522	0.2344	0.2257	0.2224	0.2213
4	0.2519	0.2341	0.2253	0.2221	0.2211	4	0.2518	0.2340	0.2252	0.2221	0.2210
5	0.2518	0.2340	0.2252	0.2221	0.2210	5	0.2518	0.2340	0.2252	0.2220	0.2210
6	0.2518	0.2340	0.2252	0.2220	0.2210	6	0.2518	0.2340	0.2252	0.2220	0.2210
7	0.2518	0.2340	0.2252	0.2220	0.2210	7	0.2518	0.2340	0.2252	0.2220	0.2210
8	0.2518	0.2340	0.2252	0.2220	0.2210	8	0.2518	0.2340	0.2252	0.2220	0.2210

$$\theta = \pi/2$$

$$|\mathcal{R}_{2,k}| \approx 0.2208$$

TABLE 2. Top: Two ellipsoids S_1 and S_2 with radii $R_1 = R_2 = (1, 1/2, 1/2)$ and centers $C_1 = (0, -1/4, 0)$ and $C_2 = (0, 1, 0)$; Bottom: S_1 is kept fixed and S_2 is rotated in the counter-clockwise direction by $\pi/2$; $\alpha = (0, 0, -1)$.

$$\|\eta_{2m+2}(x)/\eta_{2m}(x) - e^{2ikd}R_\theta\|_{L_\infty(\partial S_i)}$$

$\mathcal{R}_{2,k} = e^{2ikd}R_\theta$	$K_0 = S_1$				$K_0 = S_2$			
	m	$k = 4$	$k = 8$	$k = 16$	m	$k = 4$	$k = 8$	$k = 16$
$\theta = 0$ $R_\theta \approx 0.23285$	1	0.2063	0.3430	1.1484	1	0.2104	0.3436	1.1484
	2	0.0730	0.0826	0.2308	2	0.0730	0.0826	0.2309
	3	0.0537	0.0389	0.0413	3	0.0537	0.0389	0.0413
	4	0.0504	0.0320	0.0208	4	0.0504	0.0320	0.0208
	5	0.0499	0.0309	0.0177	5	0.0499	0.0309	0.0177
	6	0.0498	0.0308	0.0172	6	0.0498	0.0308	0.0172
	7	0.0498	0.0307	0.0172	7	0.0497	0.0307	0.0172
	8	0.0498	0.0307	0.0171	8	0.0498	0.0307	0.0171
$\theta = \pi/6$ $R_\theta \approx 0.22949$	m	$k = 4$	$k = 8$	$k = 16$	m	$k = 4$	$k = 8$	$k = 16$
	1	0.1929	0.3250	1.5229	1	0.2571	0.4403	2.3092
	2	0.0829	0.0946	0.2172	2	0.0864	0.1136	0.4158
	3	0.0857	0.0479	0.0503	3	0.0578	0.0477	0.1051
	4	0.0524	0.0359	0.0344	4	0.0516	0.0349	0.0385
	5	0.0504	0.0323	0.0241	5	0.0501	0.0317	0.0231
	6	0.0497	0.0311	0.0195	6	0.0496	0.0310	0.0188
	7	0.0494	0.0312	0.0178	7	0.0494	0.0310	0.0175
8	0.0494	0.0306	0.0172	8	0.0493	0.0307	0.0171	
$\theta = \pi/4$ $R_\theta \approx 0.22639$	m	$k = 4$	$k = 8$	$k = 16$	m	$k = 4$	$k = 8$	$k = 16$
	1	0.2047	0.2870	0.9550	1	0.2823	0.4864	2.1022
	2	0.0861	0.1005	0.1450	2	0.0945	0.1260	0.3676
	3	0.0591	0.0489	0.0565	3	0.0597	0.0521	0.0935
	4	0.0521	0.0357	0.0345	4	0.0517	0.0356	0.0371
	5	0.0500	0.0320	0.0237	5	0.0497	0.0317	0.0227
	6	0.0493	0.0307	0.0191	6	0.0492	0.0309	0.0185
	7	0.0491	0.0309	0.0175	7	0.0490	0.0306	0.0173
8	0.0490	0.0303	0.0170	8	0.0490	0.0303	0.0169	
$\theta = \pi/3$ $R_\theta \approx 0.22349$	m	$k = 4$	$k = 8$	$k = 16$	m	$k = 4$	$k = 8$	$k = 16$
	1	0.2084	0.2898	0.4905	1	0.3087	0.5206	1.7528
	2	0.0857	0.0990	0.1423	2	0.0991	0.1343	0.3887
	3	0.0581	0.0469	0.0555	3	0.0604	0.0534	0.0979
	4	0.0513	0.0344	0.0307	4	0.0515	0.0355	0.0363
	5	0.0494	0.0313	0.0214	5	0.0493	0.0313	0.0215
	6	0.0488	0.0309	0.0181	6	0.0488	0.0304	0.0178
	7	0.0487	0.0302	0.0170	7	0.0487	0.0301	0.0169
8	0.0486	0.0299	0.0167	8	0.0486	0.0299	0.0166	
$\theta = \pi/2$ $R_\theta \approx 0.22349$	m	$k = 4$	$k = 8$	$k = 16$	m	$k = 4$	$k = 8$	$k = 16$
	1	0.2062	0.2851	0.3723	1	0.3087	0.4921	0.9854
	2	0.0830	0.0931	0.1316	2	0.1016	0.1390	0.3005
	3	0.0562	0.0434	0.0419	3	0.0601	0.0534	0.0830
	4	0.0502	0.0326	0.0219	4	0.0510	0.0349	0.0311
	5	0.0487	0.0303	0.0176	5	0.0490	0.0308	0.0196
	6	0.0484	0.0302	0.0166	6	0.0485	0.0298	0.0171
	7	0.0483	0.0298	0.0164	7	0.0483	0.0296	0.0165
8	0.0483	0.0296	0.0164	8	0.0484	0.0295	0.0164	

TABLE 3. Two ellipsoids S_1 and S_2 given by (5.5): S_1 is kept fixed, and S_2 is rotated about the y -axis by $0, \pi/6, \pi/4, \pi/3, \pi/2$ in the counter-clockwise direction; $\alpha = (0, 0, -1)$.

APPENDIX A. DERIVATIVES OF PHASE FUNCTIONS

In this appendix we collect some detailed properties of the phase functions (2.24), particularly on their derivatives, that are used in Sect. 3 to derive the asymptotic expression (3.2). More precisely, these derivations necessitate expressions for the first and second derivatives of the phase function

$$(A.1) \quad \Phi(x^{m+1}; x^m) = |x^{m+1} - x^m| + \varphi_m(x^m) = \alpha \cdot x^0 + \sum_{j=0}^m |x^{j+1} - x^j|, \quad x^m \in \partial K_m$$

where x^{m+1} is an arbitrary but *fixed* point on ∂K_{m+1} , φ_m is given by (2.24), and $(x^0, \dots, x^m) \in \partial K_0 \times \dots \times \partial K_m$ denotes the broken $(m+1)$ -ray terminating at $x^m \in \partial K_m$. To this end, we consider the *local* parametrizations $x^m = x^m(t_1^m, t_2^m)$ of the surfaces ∂K_m where

$$x_{t_p^m}^m = \frac{\partial}{\partial t_p^m} x^m(t_1^m, t_2^m) \quad \text{for } p = 1, 2$$

are the principal directions at x^m . Note that, in local coordinates, we have $\Phi(x^{m+1}; x^m) = \Phi(x^{m+1}; t_1^m, t_2^m)$ and the next lemma provides explicit expressions for the first order partial derivatives.

Lemma A.1 (Partial derivatives). *In local coordinates, the partial derivatives of the phase functions (A.1) are given by*

$$(A.2) \quad \frac{\partial \Phi(x^1; x^0)}{\partial t_p^0} = \left(\alpha - \frac{x^1 - x^0}{|x^1 - x^0|} \right) \cdot x_{t_p^0}^0$$

and

$$(A.3) \quad \frac{\partial \Phi(x^{m+1}; x^m)}{\partial t_p^m} = \left(\frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} - \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} \right) \cdot x_{t_p^m}^m, \quad m \geq 1.$$

Proof. The proof of (A.2) is straightforward. For $m \geq 1$, we differentiate (A.1) with respect to t_p^m to obtain

$$\begin{aligned} \frac{\partial \Phi(x^{m+1}; x^m)}{\partial t_p^m} &= \left(\alpha - \frac{x^1 - x^0}{|x^1 - x^0|} \right) \cdot \sum_{r=1}^2 x_{t_r^0}^0 \frac{\partial t_r^0}{\partial t_p^m} + \sum_{j=0}^{m-2} \left(\frac{x^{j+1} - x^j}{|x^{j+1} - x^j|} - \frac{x^{j+2} - x^{j+1}}{|x^{j+2} - x^{j+1}|} \right) \cdot \sum_{r=1}^2 x_{t_r^{j+1}}^{j+1} \frac{\partial t_r^{j+1}}{\partial t_p^m} \\ &\quad + \left(\frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} - \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} \right) \cdot \sum_{r=1}^2 x_{t_r^m}^m \frac{\partial t_r^m}{\partial t_p^m} \end{aligned}$$

which reduces to (A.3) since (x^0, \dots, x^m) is the broken $(m+1)$ -ray terminating at x^m . \square

The next result states that $\Phi(x^{m+1}; x^m)$ is stationary at a point x^m if and only if the tuple $(x^0, \dots, x^m, x^{m+1})$ is the broken $(m+2)$ -ray terminating at x^{m+1} .

Lemma A.2. i) Stationary points in first reflections: *For $m = 0$, the phase (A.1) is stationary at a point x^0 if and only if*

$$(A.4) \quad \frac{x^1 - x^0}{|x^1 - x^0|} = \alpha + 2 \frac{x^1 - x^0}{|x^1 - x^0|} \cdot \nu_0 \nu_0$$

or

$$(A.5) \quad \frac{x^1 - x^0}{|x^1 - x^0|} = \alpha$$

ii) Stationary points in further reflections: *For $m \geq 1$, the phase (A.1) is stationary at a point x^m if and only if*

$$(A.6) \quad \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} = \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} + 2 \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} \cdot \nu_m \nu_m$$

or

$$(A.7) \quad \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} = \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|}$$

Proof. Lemma A.1 implies that $\Phi(x^1; x^0)$ has a vanishing gradient at x^0 if and only if

$$\alpha - \frac{x^1 - x^0}{|x^1 - x^0|} = \lambda_0 \nu_0$$

for some λ_0 . Also, since $|\alpha| = 1$, we have

$$1 = \alpha \cdot \alpha = \lambda_0^2 + 2\lambda_0 \frac{x^1 - x^0}{|x^1 - x^0|} \cdot \nu_0 + 1$$

so that

$$\lambda_0 = -2 \frac{x^1 - x^0}{|x^1 - x^0|} \cdot \nu_0 \quad \text{or} \quad \lambda_0 = 0.$$

Similarly, for $m \geq 1$, $\Phi(x^{m+1}; x^m)$ has a vanishing gradient at x^m if and only if

$$\frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} - \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} = \lambda_m \nu_m$$

for some λ_m . Since

$$1 = \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} \cdot \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} = \lambda_m^2 + 2\lambda_m \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} \cdot \nu_m + 1$$

we get

$$\lambda_m = -2 \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} \cdot \nu_m \quad \text{or} \quad \lambda_m = 0$$

completing the proof. \square

The derivations in Sect 3 further demand the evaluation of the Hessians of the phase (A.1) at the stationary points as derived in Lemma A.2. We note, however, that the conditions (A.5) and (A.7) cannot hold under the no-occlusion and visibility assumptions. Our next result then provides an expression for the Hessians at the points characterized by (A.4) and (A.6). It shows, in particular, that

$$(A.8) \quad N_m^m = |x^m - x^{m-1}| H_m$$

where $H_m \in \mathbb{R}^{2 \times 2}$ is defined for $m \geq 1$ by

$$(A.9) \quad (H_m)_{pq} = \frac{1}{|x_{t_p}^{m-1}| |x_{t_q}^{m-1}|} \frac{\partial^2 \Phi(x^m; x^{m-1})}{\partial t_p^{m-1} \partial t_q^{m-1}};$$

equations (A.8)–(A.9), in turn, yield for $m \geq 1$

$$\det N_m^m = |x^m - x^{m-1}|^2 \det(\text{Hess}[\Phi(x^m; x^{m-1})]) \prod_{r=1}^2 |x_{t_r}^{m-1}|^{-2}.$$

Remark A.3. Since $\{x_{t_p}^m\}_{p=1,2}$ are the principal directions, we have

$$x_{t_p}^m \cdot \nu_m = -(\kappa_m)_{pq} |x_{t_p}^m| |x_{t_q}^m|.$$

Theorem A.4. (i) (Hessians in first reflections) For $m = 0$, if (A.4) holds, then

$$(A.10) \quad H_1 = 2 \frac{x^1 - x^0}{|x^1 - x^0|} \cdot \nu_0 \kappa_0 + \frac{1}{|x^1 - x^0|} U_0.$$

(ii) (Hessians in further reflections) For $m \geq 1$, if (A.6) holds, then

$$(A.11) \quad H_{m+1} = 2 \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} \cdot \nu_m \kappa_m + \left(\frac{1}{|x^{m+1} - x^m|} + \frac{1}{|x^m - x^{m-1}|} \right) U_m - T_{m-1} H_m^{-1} T_{m-1}^t$$

Proof. Differentiating the identity

$$\left(\alpha - \frac{x^1 - x^0}{|x^1 - x^0|} \right) \cdot x_{t_p^0}^0 = 0$$

with respect to t_q^0 yields

$$\frac{\partial^2 \Phi(x^1; x^0)}{\partial t_p^0 \partial t_q^0} = \left(\alpha - \frac{x^1 - x^0}{|x^1 - x^0|} \right) \cdot x_{t_p^0 t_q^0}^0 + \frac{|x_{t_p^0}^0| |x_{t_q^0}^0|}{|x^1 - x^0|} (U_0)_{pq} = -2 \frac{x^1 - x^0}{|x^1 - x^0|} \cdot \nu_0 x_{t_p^0 t_q^0}^0 \cdot \nu_0 + \frac{|x_{t_p^0}^0| |x_{t_q^0}^0|}{|x^1 - x^0|} (U_0)_{pq}.$$

Therefore (A.10) follows from Remark A.3.

To prove the result for further reflections we need several additional lemmas. To this end, we introduce $D_m \in \mathbb{R}^{2 \times 2}$ by setting

$$(D_m)_{pq} = \frac{|x_{t_p^{m-1}}^{m-1}|}{|x_{t_q^m}^m|} \frac{\partial t_p^{m-1}}{\partial t_q^m}, \quad m \geq 1.$$

Lemma A.5. *For $m \geq 1$, if (A.6) holds, then*

$$H_{m+1} = 2 \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} \cdot \nu_m \kappa_m + \left(\frac{1}{|x^{m+1} - x^m|} + \frac{1}{|x^m - x^{m-1}|} \right) U_m - \frac{1}{|x^m - x^{m-1}|} T_{m-1} D_m.$$

Proof. Differentiating the identity

$$\left(\frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} - \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} \right) \cdot x_{t_p^m}^m = 0$$

with respect to t_q^m yields

$$\begin{aligned} \frac{\partial^2 \Phi(x^{m+1}; x^m)}{\partial t_p^m \partial t_q^m} &= \left(\frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} - \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} \right) \cdot x_{t_p^m t_q^m}^m + \frac{|x_{t_p^m}^m| |x_{t_q^m}^m|}{|x^m - x^{m-1}|} F \left(\frac{x_{t_p^m}^m}{|x_{t_p^m}^m|}, \frac{x_{t_q^m}^m}{|x_{t_q^m}^m|}, \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} \right) \\ &+ \frac{|x_{t_p^m}^m| |x_{t_q^m}^m|}{|x^{m+1} - x^m|} F \left(\frac{x_{t_p^m}^m}{|x_{t_p^m}^m|}, \frac{x_{t_q^m}^m}{|x_{t_q^m}^m|}, \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} \right) - \sum_{r=1}^2 \frac{|x_{t_p^m}^m| |x_{t_r^{m-1}}^{m-1}|}{|x^m - x^{m-1}|} F \left(\frac{x_{t_p^m}^m}{|x_{t_p^m}^m|}, \frac{x_{t_r^{m-1}}^{m-1}}{|x_{t_r^{m-1}}^{m-1}|}, \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} \right) \frac{\partial t_r^{m-1}}{\partial t_q^m}. \end{aligned}$$

Using (A.6), we therefore obtain

$$\begin{aligned} \frac{\partial^2 \Phi(x^{m+1}; x^m)}{\partial t_p^m \partial t_q^m} &= -2 \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} \cdot \nu_m x_{t_p^m t_q^m}^m \cdot \nu_m + \frac{|x_{t_p^m}^m| |x_{t_q^m}^m|}{|x^m - x^{m-1}|} F \left(\frac{x_{t_p^m}^m}{|x_{t_p^m}^m|}, \frac{x_{t_q^m}^m}{|x_{t_q^m}^m|}, \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} \right) \\ &+ \frac{|x_{t_p^m}^m| |x_{t_q^m}^m|}{|x^{m+1} - x^m|} F \left(\frac{x_{t_p^m}^m}{|x_{t_p^m}^m|}, \frac{x_{t_q^m}^m}{|x_{t_q^m}^m|}, \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} \right) - \sum_{r=1}^2 \frac{|x_{t_p^m}^m| |x_{t_r^{m-1}}^{m-1}|}{|x^m - x^{m-1}|} F \left(\frac{x_{t_p^m}^m}{|x_{t_p^m}^m|}, \frac{x_{t_r^{m-1}}^{m-1}}{|x_{t_r^{m-1}}^{m-1}|}, \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} \right) \frac{\partial t_r^{m-1}}{\partial t_q^m}. \end{aligned}$$

Thus, we get by Remark A.3

$$\begin{aligned} (H_{m+1})_{pq} &= 2 \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} \cdot \nu_m (\kappa_m)_{pq} + \left(\frac{1}{|x^{m+1} - x^m|} + \frac{1}{|x^m - x^{m-1}|} \right) F \left(\frac{x_{t_p^m}^m}{|x_{t_p^m}^m|}, \frac{x_{t_q^m}^m}{|x_{t_q^m}^m|}, \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} \right) \\ &- \frac{1}{|x^m - x^{m-1}|} \sum_{r=1}^2 F \left(\frac{x_{t_p^m}^m}{|x_{t_p^m}^m|}, \frac{x_{t_r^{m-1}}^{m-1}}{|x_{t_r^{m-1}}^{m-1}|}, \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} \right) \frac{|x_{t_r^{m-1}}^{m-1}|}{|x_{t_q^m}^m|} \frac{\partial t_r^{m-1}}{\partial t_q^m} \end{aligned}$$

or equivalently

$$\begin{aligned} (H_{m+1})_{pq} &= 2 \frac{x^{m+1} - x^m}{|x^{m+1} - x^m|} \cdot \nu_m (\kappa_m)_{pq} + \left(\frac{1}{|x^{m+1} - x^m|} + \frac{1}{|x^m - x^{m-1}|} \right) (U_m)_{pq} \\ &- \frac{1}{|x^m - x^{m-1}|} \sum_{r=1}^2 (T_{m-1})_{pr} (D_m)_{rq} \end{aligned}$$

completing the proof. \square

In light of Lemma A.5, to complete the proof of (A.11) and therefore of Theorem A.4 it suffices to show:

Lemma A.6. For $m \geq 1$, we have

$$H_m D_m = \frac{1}{|x^m - x^{m-1}|} T_{m-1}^t.$$

Proof. Differentiating the identity

$$\left(\alpha - \frac{x^1 - x^0}{|x^1 - x^0|} \right) \cdot x_{t_p^0}^0 = 0$$

with respect to t_q^1 yields

$$\begin{aligned} 0 = & \left(\alpha - \frac{x^1 - x^0}{|x^1 - x^0|} \right) \cdot \left(\sum_{r=1}^2 x_{t_p^0 t_r^0}^0 \frac{\partial t_r^0}{\partial t_q^1} \right) + \sum_{r=1}^2 \frac{|x_{t_p^0}^0| |x_{t_r^0}^0|}{|x^1 - x^0|} F \left(\frac{x_{t_p^0}^0}{|x_{t_p^0}^0|}, \frac{x_{t_r^0}^0}{|x_{t_r^0}^0|}, \frac{x^1 - x^0}{|x^1 - x^0|} \right) \frac{\partial t_r^0}{\partial t_q^1} \\ & - \frac{|x_{t_q^1}^1| |x_{t_p^0}^0|}{|x^1 - x^0|} F \left(\frac{x_{t_q^1}^1}{|x_{t_q^1}^1|}, \frac{x_{t_p^0}^0}{|x_{t_p^0}^0|}, \frac{x^1 - x^0}{|x^1 - x^0|} \right) \end{aligned}$$

so that

$$\begin{aligned} -2 \frac{x^1 - x^0}{|x^1 - x^0|} \cdot \nu_0 \left(\sum_{r=1}^2 x_{t_p^0 t_r^0}^0 \frac{\partial t_r^0}{\partial t_q^1} \right) \cdot \nu_0 + \sum_{r=1}^2 \frac{|x_{t_p^0}^0| |x_{t_r^0}^0|}{|x^1 - x^0|} F \left(\frac{x_{t_p^0}^0}{|x_{t_p^0}^0|}, \frac{x_{t_r^0}^0}{|x_{t_r^0}^0|}, \frac{x^1 - x^0}{|x^1 - x^0|} \right) \frac{\partial t_r^0}{\partial t_q^1} \\ = \frac{|x_{t_q^1}^1| |x_{t_p^0}^0|}{|x^1 - x^0|} F \left(\frac{x_{t_q^1}^1}{|x_{t_q^1}^1|}, \frac{x_{t_p^0}^0}{|x_{t_p^0}^0|}, \frac{x^1 - x^0}{|x^1 - x^0|} \right); \end{aligned}$$

therefore, Remark A.3 gives

$$2 \frac{x^1 - x^0}{|x^1 - x^0|} \cdot \nu_0 \sum_{r=1}^2 (\kappa_0)_{pr} (D_1)_{rq} + \frac{1}{|x^1 - x^0|} \sum_{r=1}^2 (U_0)_{pr} (D_1)_{rq} = \frac{1}{|x^1 - x^0|} (T_0^t)_{pq}$$

proving the lemma for $m = 1$. For $m > 1$, first we differentiate the identity

$$\left(\frac{x^{m-1} - x^{m-2}}{|x^{m-1} - x^{m-2}|} - \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} \right) \cdot x_{t_p^{m-1}}^{m-1} = 0$$

with respect to t_q^m to get

$$\begin{aligned} 0 = & \left(\frac{x^{m-1} - x^{m-2}}{|x^{m-1} - x^{m-2}|} - \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} \right) \cdot \left(\sum_{r=1}^2 x_{t_p^{m-1} t_r^{m-1}}^{m-1} \frac{\partial t_r^{m-1}}{\partial t_q^m} \right) \\ & + \sum_{r=1}^2 \frac{|x_{t_p^{m-1}}^{m-1}| |x_{t_r^{m-1}}^{m-1}|}{|x^{m-1} - x^{m-2}|} F \left(\frac{x_{t_p^{m-1}}^{m-1}}{|x_{t_p^{m-1}}^{m-1}|}, \frac{x_{t_r^{m-1}}^{m-1}}{|x_{t_r^{m-1}}^{m-1}|}, \frac{x^{m-1} - x^{m-2}}{|x^{m-1} - x^{m-2}|} \right) \frac{\partial t_r^{m-1}}{\partial t_q^m} \\ & + \sum_{r=1}^2 \frac{|x_{t_p^{m-1}}^{m-1}| |x_{t_r^{m-1}}^{m-1}|}{|x^m - x^{m-1}|} F \left(\frac{x_{t_p^{m-1}}^{m-1}}{|x_{t_p^{m-1}}^{m-1}|}, \frac{x_{t_r^{m-1}}^{m-1}}{|x_{t_r^{m-1}}^{m-1}|}, \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} \right) \frac{\partial t_r^{m-1}}{\partial t_q^m} \\ & - \sum_{r=1}^2 \frac{|x_{t_p^{m-1}}^{m-1}| |x_{t_r^{m-2}}^{m-2}|}{|x^{m-1} - x^{m-2}|} F \left(\frac{x_{t_p^{m-1}}^{m-1}}{|x_{t_p^{m-1}}^{m-1}|}, \frac{x_{t_r^{m-2}}^{m-2}}{|x_{t_r^{m-2}}^{m-2}|}, \frac{x^{m-1} - x^{m-2}}{|x^{m-1} - x^{m-2}|} \right) \frac{\partial t_r^{m-2}}{\partial t_q^m} \\ & - \frac{|x_{t_p^{m-1}}^{m-1}| |x_{t_q^m}^m|}{|x^m - x^{m-1}|} F \left(\frac{x_{t_q^m}^m}{|x_{t_q^m}^m|}, \frac{x_{t_p^{m-1}}^{m-1}}{|x_{t_p^{m-1}}^{m-1}|}, \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} \right); \end{aligned}$$

to simplify this equation, we apply the identity

$$(A.12) \quad \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} = \frac{x^{m-1} - x^{m-2}}{|x^{m-1} - x^{m-2}|} + 2 \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} \cdot \nu_{m-1} \nu_{m-1}$$

in conjunction with Remark A.3 to the first term on the right-hand side; use (A.12) to combine the second and third terms; divide the equation by the product $|x_{t_p}^{m-1}| |x_{t_q}^m|$; and finally apply the chain rule to $\partial t_r^{m-2}/\partial t_q^m$ in the fourth term. These deliver the alternate equation

$$\begin{aligned}
& 2 \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} \cdot \nu_{m-1} \sum_{r=1}^2 (\kappa_{m-1})_{pr} (D_m)_{rq} \\
& + \left(\frac{1}{|x^m - x^{m-1}|} + \frac{1}{|x^{m-1} - x^{m-2}|} \right) \times \sum_{r=1}^2 F \left(\frac{x_{t_p}^{m-1}}{|x_{t_p}^{m-1}|}, \frac{x_{t_r}^{m-1}}{|x_{t_r}^{m-1}|}, \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} \right) \left(\frac{|x_{t_r}^{m-1}|}{|x_{t_q}^m|} \frac{\partial t_r^{m-1}}{\partial t_q^m} \right) \\
& - \frac{1}{|x^{m-1} - x^{m-2}|} \sum_{s=1}^2 \sum_{r=1}^2 F \left(\frac{x_{t_p}^{m-1}}{|x_{t_p}^{m-1}|}, \frac{x_{t_r}^{m-2}}{|x_{t_r}^{m-2}|}, \frac{x^{m-1} - x^{m-2}}{|x^{m-1} - x^{m-2}|} \right) \times \left(\frac{|x_{t_r}^{m-2}|}{|x_{t_s}^{m-1}|} \frac{\partial t_r^{m-2}}{\partial t_s^{m-1}} \right) \left(\frac{|x_{t_s}^{m-1}|}{|x_{t_q}^m|} \frac{\partial t_s^{m-1}}{\partial t_q^m} \right) \\
& = \frac{1}{|x^m - x^{m-1}|} F \left(\frac{x_{t_q}^m}{|x_{t_q}^m|}, \frac{x_{t_p}^{m-1}}{|x_{t_p}^{m-1}|}, \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} \right),
\end{aligned}$$

or equivalently

$$\begin{aligned}
& 2 \frac{x^m - x^{m-1}}{|x^m - x^{m-1}|} \cdot \nu_{m-1} \sum_{r=1}^2 (\kappa_{m-1})_{pr} (D_m)_{rq} + \left(\frac{1}{|x^m - x^{m-1}|} + \frac{1}{|x^{m-1} - x^{m-2}|} \right) \sum_{r=1}^2 (U_{m-1})_{pr} (D_m)_{rq} \\
& - \frac{1}{|x^{m-1} - x^{m-2}|} \sum_{s=1}^2 \sum_{r=1}^2 (T_{m-2})_{pr} (D_{m-1})_{rs} (D_m)_{sq} = \frac{1}{|x^m - x^{m-1}|} (T_{m-1})_{pq}
\end{aligned}$$

which completes the proof of the lemma and of Theorem A.4. \square

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