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Metasurfaces and Optimal transport

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Abstract. This paper provides a theoretical and numerical approach to show existence, uniqueness, and the numerical determination of metalenses refracting radiation with energy patterns. The theoretical part uses ideas from optimal transport and for the numerical solution we study and implement a damped Newton algorithm to solve the semi discrete problem. A detailed analysis is carried out to solve the near field one source refraction problem and extensions to the far field are also mentioned.

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1. Introduction

Metalenses or metasurfaces are ultra thin surfaces with arrangements of nano scattering structures designed to focus light in imaging. They introduce abrupt phase changes over the scale of the wavelength along the optical path to bend light in unusual ways. This is in contrast with conventional lenses, where the question is to determine its faces so that a gradual change of phase accumulates as the wave propagates inside the lens, reshaping the scattered wave at will. These nano structures are engineered by adjusting their shape, size, position and orientation, and arranged on the surface (typically a plane) in the form of tiny pillars, rings, and others dispositions, working together to manipulate light waves as they pass through. The subject of metalenses is an important area of current research, one of the nine runners-up for Science's Breakthrough of the Year 2016 [1], and is potentially useful in imaging applications. Metalenses are thinner than a sheet of paper and far lighter than glass, and they could revolutionize optical imaging devices from microscopes to virtual reality displays and cameras, including the ones in smartphones; see [1], [3], and [12].

Mathematically, a metalens can be described as pair (Γ, ϕ) , where Γ is a surface in 3-d space given by the graph of a C^2 function u , and ϕ is a function, called the *phase discontinuity*, defined in a small neighborhood of Γ . The knowledge of ϕ yields the kind of arrangements of the nano structures on the

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surface that are needed for a specific refraction job. Refraction here acts following the generalized Snell law (2.1). For example, if $\Gamma = \Pi$ is a plane and the phase ϕ has the form (2.2), then the metasurface (Γ, ϕ) refracts all rays from the origin O into the point Y .

The question considered in this paper concerns existence, uniqueness and the numerical determination of metalenses refracting radiation with energy patterns. We state the problem in the near field case; the far field is explained in Section 5. Precisely, suppose radiation is emanating from a point source O , below a given surface Γ , with intensity $f(x)$ for each $x \in \Omega$ a domain of the unit sphere S^2 . Furthermore, T is a compact set, above the surface Γ , and a distribution of energy on T is given by a Radon measure μ so that $\int_{\Omega} f(x) dx = \mu(T)$. We denote $\mathcal{T}(E)$ (see Definition 2.2) the collection of points in Ω that are refracted into E in accordance with the generalized Snell law (2.1). Then, under what circumstances is there a phase discontinuity function ϕ defined in a neighborhood of Γ so that the metalens (Γ, ϕ) refracts Ω into T and satisfies the energy conservation

$$\int_{\mathcal{T}(E)} f(x) dx = \mu(E)$$

for each $E \subset T$? We will solve this problem using ideas from optimal transport. Our first result is existence and uniqueness of solutions in the semi-discrete case, that is, when μ is a finite combination of delta functions and Γ is a plane, Theorem 2.3. A relative visibility condition between Ω and T is needed, condition (2.5), and to obtain our results we use [5]. We also provide a numerical solution of the semi-discrete problem using a damped Newton algorithm, introduced in Section 4.1. This requires a careful analysis of the refractor mapping, Definition 2.2, and the Laguerre cells in (3.1).

We mention that the phase discontinuity functions needed to design metalenses for various refraction and reflection problems with prescribed distributions of energy satisfy partial differential equations of Monge–Ampère type which are derived and studied in [6]. Equations of these type also appear naturally in solving problems involving aspherical lenses, see [4, 2, 8, 9], and references therein.

The paper is organized as follows. Section 2 contains a precise description of the problem and the existence and uniqueness results. The Laguerre cells for our problem and the analysis of the refractor mapping is the contents of Section 3. To handle the singular set (3.8) where the Laguerre cells intersect the boundary of Ω , we assume that the target T is contained in a plane parallel to the metasurface and the boundary $\partial\Omega$ is not a conic section, see Remark 3.3. In Section 4 we show that 2D Laguerre cells, which are complicated objects, can be computed in a simpler way from a 3D power diagram, a tessellation of the 3D space into convex polyhedra. This leads to an effective method to solve the near-field refractor problem, which is tested on a few cases. Finally, Section 5 contains the far field case for both collimated and point sources.

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2. Refraction from one point into a near field target

2.1. Generalized Snell’s law

Let $S \subseteq \mathbb{R}^3$ be a smooth surface defined implicitly by the equation $\psi(x) = 0$, where $x = (x_1, x_2, x_3) \in \mathbb{R}^3$, and let ϕ be a function defined in a small neighborhood of S . The region below S is made up of an homogeneous material I with refractive index n_1 , and the region above S is made up of an homogeneous material II having refractive index n_2 . From a point A in I, a wave is emitted, it strikes S at some point X , and is then transmitted to a point B in medium II. Let us fix A and B and we

want to minimize

$$n_1 |x - A| + n_2 |x - B| - \phi(x)$$

over all $x \in S$, i.e., with $\psi(x) = 0$. From the existence of Lagrange multipliers, the gradient vector $\nabla_x (n_1 |x - A| + n_2 |x - B| - \phi(x))$ must be parallel to the normal vector $\nabla\psi(x)$ at all critical points x . That is, the vector product $\nabla_x (n_1 |x - A| + n_2 |x - B| - \phi(x)) \times \nu(x) = 0$, with $\nu(x)$ being the normal to S . If we set $\mathbf{x} = \frac{x-A}{|x-A|}$, and $\mathbf{m} = \frac{B-x}{|x-B|}$, then $(n_1 \mathbf{x} - n_2 \mathbf{m} - \nabla\phi(x)) \times \nu(x) = 0$. This means the vectors are multiple one from the other, that is, we obtain the *generalized Snell law*

$$n_1 \mathbf{x} - n_2 \mathbf{m} = \lambda \nu(x) + \nabla\phi(x), \quad (2.1)$$

for some $\lambda \in \mathbb{R}$; the function ϕ is called the phase discontinuity; for a derivation of this law using wave fronts see [7].

2.2. Formulation of the problem

Let Π denote the plane $x_3 = \alpha$ in \mathbb{R}^3 , $\alpha > 0$. We assume throughout that there is vacuum below and above that plane, that is, $n_1 = n_2 = 1$. Rays emanate from the origin O with directions $x \in \Omega_0 \subset S^2$, a compact domain, and intensity $f(x)$. Given $x \in \Omega_0$, let $X \in \Pi$ so that $x = X/|X|$, and set

$$\Omega = \{X \in \Pi : X/|X| \in \Omega_0\},$$

establishing a one to one correspondence between $\Omega_0 \subset S^2$ and the compact domain $\Omega \subset \Pi$. From [7, Section 7.A], given a point Y above the plane Π , the phase discontinuity ϕ so that the metasurface (Π, ϕ) refracts rays from O into Y , with ϕ tangential to Π , i.e., $\nabla\phi(X) \cdot (0, 0, 1) = 0$, is given by

$$\phi(X) = |X| + |X - Y| := c(X, Y), \quad X \in \Pi, \quad (2.2)$$

and extended to a neighborhood of Π with $\phi(x_1, x_2, x_3) = c((x_1, x_2, \alpha), Y)$. Let T be a compact domain in \mathbb{R}^3 above the plane Π , with $\text{dist}(T, \Pi) > 0$, T is referred as the target or receiver. Next, to formulate precisely the problem we first introduce the following definitions.

Definition 2.1 (Admissible phase near field). The function $\phi : \Omega \rightarrow \mathbb{R}$ is an admissible phase refracting Ω into T if for each $X_0 \in \Omega$ there exists $b \in \mathbb{R}$ and $Y \in T$ such that

$$\phi(X) \leq c(X, Y) + b \quad \forall X \in \Omega, \quad \phi(X_0) = c(X_0, Y) + b.$$

In this case, we say that $c(X, Y) + b$ supports ϕ at X_0 .

Is easy to see that admissible phases are Lipschitz continuous, $|\phi(X) - \phi(Y)| \leq 2|X - Y|$ for all $X, Y \in \Omega$.

Definition 2.2 (Refractor mapping). If $\phi : \Omega \rightarrow \mathbb{R}$ is an admissible phase, then for each $X_0 \in \Omega$ we define the set valued mapping

$$\mathcal{N}_\phi(X_0) = \{Y \in T : \text{there exists } b \in \mathbb{R} \text{ such that } c(X, Y) + b \text{ supports } \phi \text{ at } X_0\},$$

and for each $Y \in T$ we set

$$\mathcal{T}_\phi(Y) = \mathcal{N}_\phi^{-1}(Y) = \{X \in \Omega : Y \in \mathcal{N}_\phi(X)\}.$$

\mathcal{N}_ϕ is the refractor mapping and \mathcal{T}_ϕ the tracing mapping. If $E \subset \Omega$, then

$$\mathcal{T}_\phi(E) = \bigcup_{Y \in E} \mathcal{T}_\phi(Y) = \{X \in \Omega : \mathcal{N}_\phi(x) \cap E \neq \emptyset\}.$$

Now, let $f \in L^1(\Omega_0)$ with $f > 0$ a.e., and set $\rho(X)$ to be the density induced by f for $X \in \Omega$; $\rho(X) = |X|^{-3} f(X/|X|) X \cdot e$ with $e = (0, 0, 1)$. In addition, let μ be a Radon measure in T satisfying the energy conservation condition

$$\int_{\Omega} \rho(X) dX = \mu(T). \quad (2.3)$$

The problem we consider here is that of finding an admissible phase function $\phi : \Omega \rightarrow \mathbb{R}$ so that

$$\int_{\mathcal{T}_{\phi}(E)} \rho(X) dX = \mu(E) \quad (2.4)$$

for each Borel set $E \subset T$. This means the metasurface (Ω, ϕ) refracts Ω into T satisfying the energy conservation condition (2.4). In the following section we prove existence of solutions to this problem.

In order to get existence and uniqueness of solutions, we assume that $|\partial\Omega| = 0^1$ and that the points Y_1, \dots, Y_N satisfy the following condition, which holds for instance if the target T is contained in the plane $x_3 = \beta$ with $\beta > \alpha$:

$$\forall (X, Y_1, Y_2) \in \Omega \times T \times T, \quad Y_1 \neq Y_2 \implies X, Y_1, Y_2 \text{ are not aligned.} \quad (2.5)$$

It will be proved in Section 2.3 below that (2.5) implies that \mathcal{N}_{ϕ} is single valued for almost every X .

We then have the following existence and uniqueness theorem.

Theorem 2.3. *Let Ω be a compact connected domain on the plane $\Pi = \{x_3 = \alpha\}$, $\alpha > 0$, with $|\partial\Omega| = 0$, and let Y_1, \dots, Y_N be distinct points in the target T laying above Π and satisfying (2.5) with $\text{dist}(\Omega, T) > 0$. Further, let g_1, \dots, g_N be positive numbers, and $\rho \in L^1(\Omega)$ satisfying (2.3) with the measure $\mu = \sum_{i=1}^N g_i \delta_{Y_i}$.*

Then given any $b_1 \in \mathbb{R}$, there exist unique numbers b_2, \dots, b_N such that the function

$$\phi(X) = \min_{1 \leq i \leq N} \{|X| + |X - Y_i| + b_i\} \quad (2.6)$$

solves (2.4), that is, the metasurface (Ω, ϕ) refracts Ω into T .

Remark 2.4 (Relation to optimal transport). By using Lemma 2.5 to calculate the c-transform of ϕ , one can check that the couple $(\phi, -\mathbf{b})$ constructed in Theorem 2.3 is the solution to the following maximization problem:

$$\max \left\{ \int \phi d\rho + \sum_{1 \leq i \leq N} b_i g_i : \phi \in C^0(\Omega), \mathbf{b} \in \mathbb{R}^N, \forall X \in T, \forall i \in \{1, \dots, N\}, \phi(X) + b_i \leq c(X, Y_i) \right\},$$

where $c(X, Y_i) = |X| + |X - Y_i|$. Thus, solving (2.4) amounts to solving the Kantorovich dual of the optimal transport problem

$$\min \left\{ \int c(X, Y) d\gamma(X, Y) : \gamma \in \Pi(\rho, \mu) \right\}.$$

where $\Pi(\rho, \mu)$ denotes the set of *transport plans* between ρ and μ , i.e. probability measures on $\Omega \times T$ with respective marginals ρ and μ .

¹Recall that Ω is on the plane Π , $\partial\Omega$ denotes its boundary in Π and $|\partial\Omega|$ denotes its two dimensional Lebesgue measure.

2.3. Existence of solutions

We will use the results from [5, Section 2], and we first recall some notation from there. Suppose \mathcal{X}, \mathcal{Y} are compact metric spaces and ω is a Radon measure in \mathcal{X} . $\mathcal{Y}^{\mathcal{X}}$ denotes the class of all set valued mappings $\Phi : \mathcal{X} \rightarrow \mathcal{P}(\mathcal{Y})$ that are single valued for almost all points in \mathcal{X} with respect to the measure ω . We say that $\Phi \in \mathcal{Y}^{\mathcal{X}}$ is continuous at the point $x_0 \in \mathcal{X}$ if given $x_k \rightarrow x_0$ and $y_k \in \Phi(x_k)$ there exists a subsequence y_{k_j} and $y_0 \in \Phi(x_0)$ such that $y_{k_j} \rightarrow y_0$ as $j \rightarrow \infty$. We also denote

$$C(\mathcal{X}, \mathcal{Y}) = \{\Phi \in \mathcal{Y}^{\mathcal{X}} : \Phi \text{ is continuous in } \mathcal{X}\}, \text{ and } C_s(\mathcal{X}, \mathcal{Y}) = \{\Phi \in C(\mathcal{X}, \mathcal{Y}) : \Phi(\mathcal{X}) = \mathcal{Y}\}.$$

With this set up, we let $\mathcal{X} = \Omega$, $\mathcal{Y} = T$, $\omega = \rho dx$, and to solve our problem we introduce the class

$$\mathcal{F} = \{\phi : \Omega \rightarrow \mathbb{R} : \phi \text{ is an admissible phase refracting } \Omega \text{ into } T\}.$$

From the definitions introduced above, it is easy to see that \mathcal{F} satisfies the following properties like the ones introduced in [5, Sections 2.1 and 2.3] (with the same labeling so the reader can compare):

(A1) if $\phi_1, \phi_2 \in \mathcal{F}$, then $\phi_1 \wedge \phi_2 = \min\{\phi_1, \phi_2\} \in \mathcal{F}$,

(A2) if $\phi_1(x_0) \leq \phi_2(x_0)$, then $\mathcal{N}_{\phi_1}(x_0) \subset \mathcal{N}_{\phi_1 \wedge \phi_2}(x_0)$,

(A3'') for each $Y \in T$ and each $b \in (-\infty, \infty)$, the functions $c(\cdot, Y) + b \in \mathcal{F}$ satisfy the following

(a) $Y \in \mathcal{N}_{c(\cdot, Y) + b}(X)$ for all $X \in \Omega$,

(b) $c(\cdot, Y) + b \leq c(\cdot, Y) + b'$ for all $b \leq b'$,

(c) for each $Y \in T$, $c(X, Y) + b \rightarrow +\infty$ uniformly for $X \in \Omega$ as $b \rightarrow +\infty$,

(d) for each $Y \in T$, $\max_{X \in \Omega} |c(X, Y) + b - (c(X, Y) + b')| \rightarrow 0$ as $b' \rightarrow b$.

In addition, we need to verify that

$$\mathcal{N}_{\phi} \in C_s(\Omega, T) \tag{2.7}$$

for each $\phi \in \mathcal{F}$. We first verify that $\mathcal{N}_{\phi} \in T^{\Omega}$, that is, \mathcal{N}_{ϕ} is single valued for almost all $X \in \Omega$ with respect to Lebesgue measure. Indeed, suppose that $\mathcal{N}_{\phi}(X_0)$ contains more than one point, say $Y_1, Y_2 \in \mathcal{N}_{\phi}(X_0)$ with $Y_1 \neq Y_2$ and $X_0 \in \overset{\circ}{\Omega}$. Will show that X_0 is a singular point of ϕ . We have that for some $b_1, b_2 \in \mathbb{R}$, $\phi(X) \leq |X| + |X - Y_i| + b_i$ for all $X \in \Omega$ with equality at $X = X_0$, $i = 1, 2$. Since $\text{dist}(\Omega, O) > 0$ and $\text{dist}(\Omega, T) > 0$, the support functions $|X| + |X - Y_i|$ are both smooth in the variable $X = (x_1, x_2, \alpha)$. If X_0 were not a singular point of ϕ , then ϕ has a tangent plane at X_0 which must coincide with both tangent planes to $|X| + |X - Y_i| + b_i$, $i = 1, 2$, at X_0 . So $\nabla_{x_1, x_2} (|X| + |X - Y_1|)|_{X=X_0} = \nabla_{x_1, x_2} (|X| + |X - Y_2|)|_{X=X_0}$ obtaining $\frac{X_0 - Y_1}{|X_0 - Y_1|} = \frac{X_0 - Y_2}{|X_0 - Y_2|}$ which implies that the vectors $X_0 - Y_1$ and $X_0 - Y_2$ are multiples one of the other. This contradicts (2.5) showing that X_0 is a singular point to ϕ . Since ϕ is Lipschitz, the set of points where ϕ is not differentiable has measure zero and therefore (2.5) implies that \mathcal{N}_{ϕ} is single valued for almost all $X \in \Omega$.

Second, we verify that \mathcal{N}_{ϕ} is continuous in the sense given at the beginning of this section. Indeed, let $X_k \in \Omega$ with $X_k \rightarrow X_0$, and let $Y_k \in \mathcal{N}_{\phi}(X_k)$. We then have $\phi(X) \leq c(X, Y_k) + b_k$ for all $X \in \Omega$ for some b_k with equality at $X = X_k$. Since Ω, T are compact, ϕ is continuous in Ω , and c is continuous on $\Omega \times T$, selecting subsequences is easy to obtain the desired continuity. We also have that \mathcal{N}_{ϕ} is continuous at each $\phi \in \mathcal{F}$, i.e., if $\phi_k \rightarrow \phi$ uniformly in Ω , $\phi_k \in \mathcal{F}$, $X_0 \in \Omega$ and $Y_k \in \mathcal{N}_{\phi_k}(X_0)$, then there exists a subsequence $Y_{k_j} \rightarrow Y_0 \in T$ with $Y_0 \in \mathcal{N}_{\phi}(X_0)$. In fact, there exists $b_k \in \mathbb{R}$ such that $\phi_k(X) \leq c(X, Y_k) + b_k$ for all $X \in \Omega$ with equality at $X = X_0$. That is, $b_k = \phi_k(X_0) - c(X_0, Y_k) = \phi_k(X_0) - \phi(X_0) + \phi(X_0) - c(X_0, Y_k)$, a quantity uniformly bounded in k from the uniform convergence and since Ω, T are compact. Since T is compact, there is a subsequence $Y_{k_j} \rightarrow Y_0$ for some $Y_0 \in T$, and so there is a subsequence $b_{k_{j\ell}} \rightarrow b_0$ as $\ell \rightarrow \infty$ obtaining that $c(X, Y_0) + b_0$ supports ϕ at X_0 , that is, $Y_0 \in \mathcal{N}_{\phi}(X_0)$.

To continue verifying (2.7), we next show that $\mathcal{N}_\phi(\Omega) = T$. Let $Y \in T$. Since ϕ is continuous in Ω we have

$$\phi(X) \leq \max_{\Omega} \phi \leq |X| + |X - Y| + b$$

for all $X \in \Omega$ and for $b \rightarrow \infty$. Choose

$$b_0 = \inf\{b : \phi(X) \leq |X| + |X - Y| + b, \forall X \in \Omega\}.$$

Then $\phi(X_0) = |X_0| + |X_0 - Y| + b_0$ for some $X_0 \in \Omega$, that is, $\mathcal{N}_\phi(X_0) = Y$.

To prove existence of solutions to the problem (2.4) we proceed as follows. We recall that in [5, Section 2.3] we have considered the case convex infinity. However, to show existence in the current case, we need to consider the case concave infinity which is not explicitly written in [5] but it follows along similar lines as the convex infinity case. Indeed, to obtain existence of solutions we argue as in the proof of [5, Theorem 2.12] using the family $\mathcal{F}^* = \{e^{-\phi}, \phi \in \mathcal{F}\}$ together with the mapping $\mathcal{N}_{e^{-\phi}}^* = \mathcal{N}_\phi$ which now converts the case concave-infinity into the convex case from [5, Section 2.2] with the family of supporting functions $e^{-c(X,Y)-b}$ for $b \in (-\infty, \infty)$. Hence existence in our case will follow applying [5, Theorem 2.9] with the family \mathcal{F}^* if we are under its hypotheses. That is, we need to show that there exists $(b_1^0, b_2^0, \dots, b_N^0)$ such that

$$e^{-c(X,Y_1)-b_1^0} \leq \min_{2 \leq i \leq N} e^{-c(X,Y_i)-b_i^0}$$

which is equivalent to

$$\max_{2 \leq i \leq N} c(X, Y_i) + b_i^0 \leq c(X, Y_1) + b_1^0.$$

Indeed, if b_1^0 is arbitrarily chosen then by continuity we can pick $b_2^0, \dots, b_N^0 \rightarrow -\infty$ such that the last inequality holds. Therefore, [5, Theorem 2.9] implies the existence part of Theorem 2.3.

2.4. Uniqueness of solutions to Theorem 2.3

We begin with a lemma.

Lemma 2.5. *Suppose (2.5) holds and $|\partial\Omega| = 0$. Let $\phi(X) = \min_{1 \leq i \leq N} c(X, Y_i) + b_i$ with $Y_i \in T$ distinct points. If $X \in \mathcal{T}_\phi(Y_j)$, then $c(\cdot, Y_j) + b_j$ supports ϕ at X or X belongs to the set where \mathcal{N}_ϕ is not single valued (a set of measure zero).*

Proof. Let $X \in \mathcal{T}_\phi(Y_j)$, then there exists \bar{b} such that $c(\cdot, Y_j) + \bar{b}$ supports ϕ at X . Then $c(X, Y_j) + \bar{b} = \phi(X) \leq c(X, Y_k) + b_k$ for all k , and in particular for $k = j$, so we get $\bar{b} \leq b_j$. If $\bar{b} = b_j$, then $c(\cdot, Y_j) + b_j$ supports ϕ at X . If $\bar{b} < b_j$, then $\phi(Z) \leq c(Z, Y_j) + \bar{b} < c(Z, Y_j) + b_j$ for all $Z \in \Omega$ and hence $\phi(Z) = \min_{k \neq j} c(Z, Y_k) + b_k$ for all $Z \in \Omega$. In particular, when $Z = X$, there is $k \neq j$ such that $\phi(X) = c(X, Y_k) + b_k$. This means $c(\cdot, Y_k) + b_k$ supports ϕ at X , so $X \in \mathcal{T}_\phi(Y_k)$. Hence $Y_j, Y_k \in \mathcal{N}_\phi(X)$ and so X belongs to the set where \mathcal{N}_ϕ is not single valued which is a set of measure zero. ■

For $\phi \in \mathcal{F}$, let $\mathcal{Q} = \{x \in \Omega : \mathcal{N}_\phi(x) \text{ is not singleton}\}$ which has measure zero because (2.5) holds and $|\partial\Omega| = 0$. We also have that $\mathcal{T}_\phi(K)$ is compact for each K compact subset of Ω .

Lemma 2.6. *Let $\phi(X) = \min_{1 \leq i \leq N} c(X, Y_i) + b_i$ with $Y_i \in T$ distinct points. Then for each $F \subsetneq \{Y_1, \dots, Y_N\}$, $F \neq \emptyset$ we have*

$$\partial(\mathcal{T}_\phi(F)) \subset \mathcal{Q},$$

where $\partial(\cdot)$ denotes the boundary.

Proof. Let $Z \in \partial(\mathcal{T}_\phi(F))$. Then for each $m \geq 1$ the open ball $B_{1/m}(Z)$ satisfies $B_{1/m}(Z) \cap (\mathcal{T}_\phi(F))^c \neq \emptyset$. Since $\mathcal{T}_\phi(F)$ is closed, $(\mathcal{T}_\phi(F))^c$ is open and so $B_{1/m}(Z) \cap (\mathcal{T}_\phi(F))^c$ is a non empty relatively open set and so it has positive measure for all m . Since $|\mathcal{Q}| = 0$, it follows that the set $B_{1/m}(Z) \cap (\mathcal{T}_\phi(F))^c \cap \mathcal{Q}^c$ has positive measure and we pick Z_m in that set. Hence \mathcal{N}_ϕ is single valued at Z_m , and $\mathcal{N}_\phi(Z_m) \cap F = \emptyset$. Then it follows that $\mathcal{N}_\phi(Z_m)$ can take only values in F^c , and since $\{Y_1, \dots, Y_N\}$ is a finite set there is subsequence such that $\mathcal{N}_\phi(Z_{m_j}) = Y_\ell$ for some $Y_\ell \in \{Y_1, \dots, Y_N\} \setminus F$. From Lemma 2.5, this means that $\phi(X) \leq c(X, Y_\ell) + b_\ell$ for all $X \in \Omega$ and $\phi(Z_{m_j}) = c(Z_{m_j}, Y_\ell) + b_\ell$. Since $Z_m \rightarrow Z$ as $m \rightarrow \infty$, it follows by continuity that $\phi(Z) = c(Z, Y_\ell) + b_\ell$, and so $Y_\ell \in \mathcal{N}_\phi(Z)$. On the other hand, since $Z \in \mathcal{T}_\phi(F)$ we obtain $Z \in \mathcal{Q}$. \blacksquare

We are now in a position to prove the following comparison principle, akin to [5, Theorem 2.7], which clearly implies the uniqueness in Theorem 2.3.

Proposition 2.7. *Let $\mathbf{b} = (b_1, \dots, b_N)$, $\mathbf{b}^* = (b_1^*, \dots, b_N^*)$, and let $\phi_{\mathbf{b}}, \phi_{\mathbf{b}^*}$ be given by (2.6) two admissible phases solving (2.4) with the density $\rho > 0$ a.e. and assume Ω is connected.*

If $b_1^ \geq b_1$, then $b_i^* \geq b_i$ for all $1 \leq i \leq N$. So if $b_1^* = b_1$, then $b_i^* = b_i$ for all $1 \leq i \leq N$.*

Proof. Let $I = \{i : b_i^* \geq b_i\}$ and $J = \{j : b_j > b_j^*\}$. We then want to show that $J = \emptyset$. Suppose by contradiction that $J \neq \emptyset$. From (2.4), $\int_{\mathcal{T}_{\phi_{\mathbf{b}}}(Y_i)} \rho(X) dX = g_i > 0$ for $1 \leq i \leq N$. Hence $\mathcal{T}_{\phi_{\mathbf{b}}}(Y_i)$ has positive measure for each $1 \leq i \leq N$, and likewise $\mathcal{T}_{\phi_{\mathbf{b}^*}}(Y_i)$.

Set $F = \{Y_j : j \in J\}$. We shall prove that

$$\overline{\mathcal{T}_{\phi_{\mathbf{b}}}(F)^\circ} \subset \mathcal{T}_{\phi_{\mathbf{b}^*}}(F)^\circ. \quad (2.8)$$

Let $X \in \overline{\mathcal{T}_{\phi_{\mathbf{b}}}(F)^\circ}$. We first claim that there exists $Y_j \in F$ such that $c(\cdot, Y_j) + b_j$ supports $\phi_{\mathbf{b}}$ at X . Indeed, for each $m \geq 1$, $B_{1/m}(X) \cap \mathcal{T}_{\phi_{\mathbf{b}}}(F)^\circ \neq \emptyset$, where $B_{1/m}(X)$ is the open ball with radius $1/m$ centered at X . Since the last intersection is a non empty open set, it has positive measure. Hence $|B_{1/m}(X) \cap \mathcal{T}_{\phi_{\mathbf{b}}}(F)^\circ \cap \mathcal{Q}^c| > 0$ for all m where \mathcal{Q} is the null set where $\mathcal{N}_{\phi_{\mathbf{b}}}$ is not a singleton. Let us then pick $Z_m \in B_{1/m}(X) \cap \mathcal{T}_{\phi_{\mathbf{b}}}(F)^\circ \cap \mathcal{Q}^c$ and proceed as in the proof of Lemma 2.6. That is, taking a subsequence $\mathcal{N}_{\phi_{\mathbf{b}}}(Z_{m_\ell})$ equals one value Y_j in F , so $c(\cdot, Y_j) + b_j$ supports $\phi_{\mathbf{b}}$ at Z_{m_ℓ} . Letting $\ell \rightarrow \infty$ we obtain that $c(\cdot, Y_j) + b_j$ supports $\phi_{\mathbf{b}}$ at X . The claim is then proved.

To prove (2.8), we then have

$$\begin{aligned} c(X, Y_i) + b_i^* &\geq c(X, Y_i) + b_i && \forall i \in I \\ &\geq \phi_{\mathbf{b}}(X) = c(X, Y_j) + b_j, && \text{since } X \in \overline{\mathcal{T}_{\phi_{\mathbf{b}}}(F)^\circ} \\ &> c(X, Y_j) + b_j^* && \text{since } j \in J, \end{aligned}$$

so $\min_{i \in I} c(X, Y_i) + b_i^* > c(X, Y_j) + b_j^*$. Then by continuity of c , there exists an open neighborhood N_X of the point X such that

$$\min_{i \in I} c(Z, Y_i) + b_i^* > c(Z, Y_j) + b_j^* \quad \forall Z \in N_X.$$

Hence

$$\phi_{\mathbf{b}^*}(Z) = \min_{1 \leq i \leq N} c(Z, Y_i) + b_i^* = \min_{i \in J} c(Z, Y_i) + b_i^* \quad \text{for all } Z \in N_X.$$

This implies that given $Z \in N_X$ there exists $m \in J$, depending on Z , such that $\phi_{\mathbf{b}^*}(Z) = c(Z, Y_m) + b_m^*$. By definition $\phi_{\mathbf{b}^*}(Y) \leq c(Y, Y_m) + b_m^*$ for all $Y \in \Omega$. Then $c(\cdot, Y_m) + b_m^*$ supports $\phi_{\mathbf{b}^*}$ at $Y = Z$, that is, $Z \in \mathcal{T}_{\phi_{\mathbf{b}^*}}(Y_m)$.

Therefore for each $X \in \overline{\mathcal{T}_{\phi_{\mathbf{b}}}(F)^\circ}$ there exists an open neighborhood N_X of X such that

$$N_X \subset \cup_{m \in J} \mathcal{T}_{\phi_{\mathbf{b}^*}}(Y_m) = \mathcal{T}_{\phi_{\mathbf{b}^*}}(F)$$

which proves (2.8).

Since $\mathcal{T}_{\phi_{\mathbf{b}^*}}(F)$ is closed, $\mathcal{T}_{\phi_{\mathbf{b}^*}}(F) = \mathcal{T}_{\phi_{\mathbf{b}^*}}(F)^\circ \cup \partial(\mathcal{T}_{\phi_{\mathbf{b}^*}}(F))$. Then from Lemma 2.6 and since $\rho > 0$ a.e., we obtain

$$0 < \sum_{j \in J} g_j = \int_{\mathcal{T}_{\phi_{\mathbf{b}^*}}(F)} \rho(x) dx = \int_{\mathcal{T}_{\phi_{\mathbf{b}^*}}(F)^\circ} \rho(x) dx,$$

in particular, the set $\mathcal{T}_{\phi_{\mathbf{b}^*}}(F)^\circ \neq \emptyset$. From (2.8) and connectedness of Ω , then set $\mathcal{T}_{\phi_{\mathbf{b}^*}}(F)^\circ \setminus \overline{\mathcal{T}_{\phi_{\mathbf{b}}}^\circ(F)}$ is a non empty open set and therefore it has positive measure. Obviously, $\mathcal{T}_{\phi_{\mathbf{b}}}^\circ(F) \subset \overline{\mathcal{T}_{\phi_{\mathbf{b}}}^\circ(F)}$, and so $\mathcal{T}_{\phi_{\mathbf{b}^*}}(F)^\circ \setminus \mathcal{T}_{\phi_{\mathbf{b}}}^\circ(F)$ also has positive measure. Since $\rho > 0$ a.e., we obtain

$$\int_{\mathcal{T}_{\phi_{\mathbf{b}^*}}(F)^\circ} \rho(x) dx > \int_{\mathcal{T}_{\phi_{\mathbf{b}}}^\circ(F)} \rho(x) dx$$

which is a contradiction since both sides of this inequality equal $\sum_{j \in J} g_j$. Therefore $J = \emptyset$ which completes the proof of the proposition. \blacksquare

Remark 2.8. In Definition 2.1, the admissible phase ϕ is supported by the functions $c(\cdot, \cdot) + b$ from above which yields the concave-infinity case used to prove Theorem 2.3. An alternative definition of admissible phase can be made with supporting functions $c(\cdot, \cdot) + b$ from below which yields the convex-infinity case. With this definition, proceeding in a similar way and using the results from [5, Section 2], a theorem similar to 2.3 also follows, where in (2.6) the min is replaced by max. A reason to choose the Definition 2.1, is that this notion is more suitable for the initialization of the numerical scheme developed in Section 4 to compute the Laguerre cells.

3. Analysis of the refracted distribution

Definition 3.1 (Laguerre cells and refracted distribution). We define the Laguerre cells associated to $(Y_i, b_i)_{1 \leq i \leq N}$ by

$$\text{Lag}_i(\mathbf{b}) = \{X \in \Omega : c(X, Y_i) + b_i \leq c(X, Y_k) + b_k \text{ for all } 1 \leq k \leq N\}, \quad 1 \leq i \leq N, \quad (3.1)$$

where c is given in (2.2). We call *refracted distribution* to the vector $G(\psi) \in \mathbb{R}^N$ defined by

$$G(\mathbf{b}) = (G_1(\mathbf{b}), \dots, G_N(\mathbf{b})), \quad \text{where } G_i(\mathbf{b}) = \int_{\text{Lag}_i(\mathbf{b})} \rho(X) dX, \quad (3.2)$$

which encodes the amount of light refracted in each direction $\{Y_1, \dots, Y_N\}$.

Given $\mathbf{b} = (b_1, \dots, b_N)$, let $\phi_{\mathbf{b}}$ be the function defined by (2.6), and let $\mathcal{M}_{\phi_{\mathbf{b}}}$ be the refracted measure defined by the left hand side of (2.4), that is,

$$\mathcal{M}_{\phi_{\mathbf{b}}}(E) = \int_{\mathcal{T}_{\phi_{\mathbf{b}}}(E)} \rho(X) dX.$$

One can easily verify that $\text{Lag}_i(\mathbf{b}) = \mathcal{T}_{\phi_{\mathbf{b}}}(Y_i)$, so that the refractor measure is given by

$$\mathcal{M}_{\phi_{\mathbf{b}}} = \sum_{1 \leq i \leq N} G_i(\mathbf{b}) \delta_{Y_i}.$$

Assuming that $\mu = \sum_{1 \leq i \leq N} g_i \delta_{Y_i}$ with $\mathbf{g} \in \mathbb{R}^N$, the near-field metasurface refractor problem (2.4) means to solve the finite-dimensional non-linear system of equations

$$G(\mathbf{b}) = \mathbf{g}, \quad (3.3)$$

where $\mathbf{g} = (g_1, \dots, g_N)$. The goal of this section is to gather a few properties of the refracted distribution, which will be used to establish the global convergence of a damped Newton algorithm to solve this system of equations.

3.1. Regularity of the map G

Theorem 3.2 (Partial derivatives of G). *Let $0 < \alpha < \beta$, let $\Omega \subseteq \mathbb{R}^2 \times \{\alpha\}$ be a polygon and let $\rho \in C^0(\Omega)$. Assume that the target $T = \{Y_1, \dots, Y_N\}$ is included in the plane $\{x_3 = \beta\}$. Then the refracted distribution map G given by (3.2) belongs to $C^1(\mathbb{R}^N)$ and the partial derivatives of G are given by*

$$\frac{\partial G_i}{\partial b_j}(\mathbf{b}) = G_{ij}(\mathbf{b}) := \int_{\text{Lag}_{ij}(\mathbf{b})} \frac{\rho(X)}{|\nabla_X c(X, Y_i) - \nabla_X c(X, Y_j)|} dX \quad i \neq j, \quad (3.4)$$

when $j \neq i$. where the integration is over the curve

$$\text{Lag}_{ij}(\mathbf{b}) = \text{Lag}_i(\mathbf{b}) \cap \text{Lag}_j(\mathbf{b}).$$

The diagonal partial derivatives are given by

$$\frac{\partial G_i}{\partial b_i}(\mathbf{b}) = G_{ii}(\mathbf{b}) := - \sum_{j \neq i} \frac{\partial G_i}{\partial b_j}(\mathbf{b}), \quad (3.5)$$

Remark 3.3 (Assumptions on Ω). From the proof of the theorem, one can verify that the hypothesis that Ω is a polygon can be replaced by the following two hypothesis:

- the boundary of Ω in $\mathbb{R}^2 \times \{\alpha\}$ has area zero;
- the intersection of $\partial\Omega$ with any conic in $\mathbb{R}^2 \times \{\alpha\}$ a finite set of points.

Moreover, if ρ has compact support in Ω , then the assumption that $\partial\Omega$ has measure zero is not needed.

Theorem 3.2 is proved in the same way as [13, Theorem 45], provided that we are able to show that the functions G_{ij} are continuous, which replaces [13, Lemma 46]. Note that unlike in Lemma 46, we do not need the points Y_1, \dots, Y_N to be in a generic position ([13, Definition 16]).

Lemma 3.4. *Under the assumptions of Theorem 3.2, the functions G_{ij} are continuous.*

Proof. Define $H_{ij}(\mathbf{b}) = \{X \in \Omega : c(X, Y_i) + b_i = c(X, Y_j) + b_j\}$, so that

$$\text{Lag}_{ij}(\mathbf{b}) \subset H_{ij}(\mathbf{b}), \quad (3.6)$$

$1 \leq i, j \leq N$. Set $f(X) = c(X, Y_i) - c(X, Y_j)$ for $X \in \Omega$, and let $\Omega \Subset \Omega_1 \Subset \Omega_2$ with Ω_i open sets and let \bar{f} be an extension of f to Ω_2 so that the gradient of \bar{f} is continuous in Ω_2 and agrees with the gradient of f in Ω . Consider the system of ODEs

$$\begin{cases} \frac{d\Phi}{dt}(t, X) = \frac{\nabla \bar{f}(\Phi(t, X))}{|\nabla \bar{f}(\Phi(t, X))|^2} := F(\Phi(t, X)) \\ \Phi(0, X) = X. \end{cases}$$

For ε sufficiently small, there is a unique local solution $\Phi : (-\varepsilon, \varepsilon) \times \Omega_1 \rightarrow \Omega_2$ and so that $\Phi((-\varepsilon, \varepsilon) \times \Omega) \subset \Omega_1$. Here $F(X)$ is C^1 for X in Ω_2 . Since $\frac{d}{dt} \bar{f}(\Phi(t, X)) = 1$, we have for $-\varepsilon < t < \varepsilon$ and $X \in \Omega_1$

$$\bar{f}(\Phi(t, X)) = \bar{f}(\Phi(0, X)) + t. \quad (3.7)$$

Since F is $C^1(\Omega_2)$, we also have that $\Phi(t, X) \rightarrow X$ in $C^1(\Omega_1)$ as $t \rightarrow 0$.

Now, let $\mathbf{b}^n = (b_1^n, \dots, b_N^n) \rightarrow \mathbf{b} = (b_1, \dots, b_N)$ as $n \rightarrow \infty$. We shall prove that $G_{ij}(\mathbf{b}^n) \rightarrow G_{ij}(\mathbf{b})$ as $n \rightarrow \infty$. Set

$$a := b_j - b_i, \quad t_n := b_j^n - b_i^n - a, \quad L := \text{Lag}_{ij}(\mathbf{b}), \quad L_n := \Phi(-t_n, \text{Lag}_{ij}(\mathbf{b}^n)).$$

Let $H = \bar{f}^{-1}(a) = \{X \in \Omega_1 : \bar{f}(X) = a\}$. From (3.6), $L \subset H \cap \Omega$. Also, if $X \in L_n$, there is $Y \in \text{Lag}_{ij}(\mathbf{b}^n) (\subset H_{ij}(\mathbf{b}^n))$ such that $X = \Phi(-t_n, Y)$, and from (3.7) $\bar{f}(X) = \bar{f}(Y) - t_n = b_j^n - b_i^n - t_n = a$. Since $Y \in \Omega$ we have $X \in \Omega_1$. Thus, $L_n \subset H$ for n large since $t_n \rightarrow 0$. Define for $X \in H$,

$$F_n(X) = \Phi(-t_n, X),$$

$F_n : H \rightarrow \Phi(-t_n, H) \subset \Omega_2$. We have $L_n = F_n(\text{Lag}_{ij}(\mathbf{b}^n)) \subset \Omega_1$. Write

$$\begin{aligned} G_{ij}(\mathbf{b}^n) &= \int_{\text{Lag}_{ij}(\mathbf{b}^n)} \frac{\rho(Y)}{|\nabla_X c(Y, Y_i) - \nabla_X c(Y, Y_j)|} dY \\ &= \int_{F_n^{-1}(L_n)} \frac{\rho(Y)}{|\nabla_X c(Y, Y_i) - \nabla_X c(Y, Y_j)|} dY. \end{aligned}$$

Since ρ is defined in Ω and in the last integral we will make the change of variables $Y = F_n(X)^2$, we need to extend ρ to Ω_2 , so let $\bar{\rho}$ be a bounded extension of ρ to Ω_2 so that $\bar{\rho} \in C(\Omega_2)$. So

$$\begin{aligned} G_{ij}(\mathbf{b}^n) &= \int_{L_n} \frac{\rho(F_n(X))}{|\nabla_X c(F_n(X), Y_i) - \nabla_X c(F_n(X), Y_j)|} |J_{F_n}(X)| dX \\ &= \int_H \frac{\bar{\rho}(F_n(X))}{|\nabla_X c(F_n(X), Y_i) - \nabla_X c(F_n(X), Y_j)|} |J_{F_n}(X)| \chi_{L_n}(X) dX. \end{aligned}$$

Now $F_n(X) \rightarrow \Phi(0, X) = X$ and $|J_{F_n}(X)| \rightarrow 1$ as $n \rightarrow \infty$. Hence to show that $G_{ij}(\mathbf{b}^n) \rightarrow G_{ij}(\mathbf{b})$, is enough to show that $\chi_{L_n}(X) \rightarrow \chi_L(X)$ for a.e. X . Given an arbitrary sequence of sets E_n we have the following

$$\begin{aligned} \limsup_{k \rightarrow \infty} E_k &= \bigcap_{n=1}^{\infty} \bigcup_{k \geq n} E_k \\ \liminf_{k \rightarrow \infty} E_k &= \bigcup_{n=1}^{\infty} \bigcap_{k \geq n} E_k \\ \chi_{\limsup_{k \rightarrow \infty} E_k}(X) &= \limsup_{n \rightarrow \infty} \chi_{E_n}(X) \\ \chi_{\liminf_{k \rightarrow \infty} E_k}(X) &= \liminf_{n \rightarrow \infty} \chi_{E_n}(X). \end{aligned}$$

We first prove that $\chi_{\limsup_{n \rightarrow \infty} L_n}(X) \leq \chi_L(X)$, which is equivalent to show that $\limsup_{n \rightarrow \infty} L_n \subset L$. In fact, if $X \in \limsup_{n \rightarrow \infty} L_n$, there exists a subsequence n_ℓ such that $X \in L_{n_\ell}$ for $\ell = 1, 2, \dots$. So $X = \Phi(-t_{n_\ell}, Z_{n_\ell})$ for some $Z_{n_\ell} \in \text{Lag}_{ij}(\mathbf{b}^{n_\ell})$. Since Ω is compact, there is a subsequence $Z_{n_{\ell_m}} \rightarrow Z \in \text{Lag}_{ij}(\mathbf{b}) = L$. Hence $X = \Phi(0, Z) = Z$, so $X \in L$ as desired.

Let

$$S = \bigcup_{k \neq i, j} H_{ijk}(\mathbf{b}) \cup (\text{Lag}_{ij}(\mathbf{b}) \cap \partial\Omega). \quad (3.8)$$

Under the assumptions on the boundary $\partial\Omega$ described below, we shall prove in a moment that this is a set of linear measure zero. Taking this for granted, we claim that

$$L \subset \left(\liminf_{n \rightarrow \infty} L_n \right) \cup S \quad (3.9)$$

obtaining $\chi_L(X) \leq \liminf_{n \rightarrow \infty} \chi_{L_n}(X)$ for $X \notin S$. Therefore the sequence $\chi_{L_n}(X) \rightarrow \chi_L(X)$ for a.e. X . Since $\bar{\rho}$ is continuous and bounded, we then obtain by Lebesgue dominated convergence theorem that

$$\begin{aligned} G_{ij}(\mathbf{b}^n) &= \int_H \frac{\bar{\rho}(F_n(X))}{|\nabla_X c(F_n(X), Y_i) - \nabla_X c(F_n(X), Y_j)|} |J_{F_n}(X)| \chi_{L_n}(X) dX \\ &\rightarrow \int_H \frac{\bar{\rho}(X)}{|\nabla_X c(X, Y_i) - \nabla_X c(X, Y_j)|} \chi_L(X) dX = G_{ij}(\mathbf{b}) \end{aligned}$$

²We notice that F_n is a genuine change of variables because letting $\frac{\partial\Phi}{\partial X}(t, X)$ being the Jacobian matrix of Φ , setting $J(t, X) = \det\left(\frac{\partial\Phi}{\partial X}(t, X)\right)$ we have that J satisfies the following ode:

$$\frac{\partial J}{\partial t}(t, X) = \text{div}(F)(\Phi(t, X)) J(t, X)$$

with the initial condition $J(0, X) = 1$.

as $n \rightarrow \infty$ showing that G_{ij} is continuous.

It then remains to prove the claim (3.9). Indeed, if $X \in L$ and $X \in \partial\Omega$, then $X \in S$. On the other hand, if $X \in L \cap \text{interior}(\Omega)$, and $X \notin S$, then we show $X \in \liminf_{n \rightarrow \infty} L_n$. We have

$$X \in S^c = \bigcap_{k \neq i, j} H_{ijk}(\mathbf{b})^c \cap \left(\text{Lag}_{ij}(\mathbf{b}) \cap \partial\Omega \right)^c.$$

Since $H_{ijk}(\mathbf{b}) = H_{ij}(\mathbf{b}) \cap H_{ik}(\mathbf{b})$, we then have

$$X \in \bigcap_{k \neq i, j} (H_{ij}(\mathbf{b})^c \cup H_{ik}(\mathbf{b})^c) = H_{ij}(\mathbf{b})^c \cup \bigcap_{k \neq i, j} H_{ik}(\mathbf{b})^c.$$

Since $X \in L = \text{Lag}_{ij}(\mathbf{b}) \subset H_{ij}(\mathbf{b})$, we get

$$X \in \bigcap_{k \neq i, j} H_{ik}(\mathbf{b})^c,$$

that is, $c(X, Y_i) - c(X, Y_k) \neq b_k - b_i$ for all $k \neq i$. On the other hand, since $X \in \text{Lag}_i(\mathbf{b})$ we have $c(X, Y_i) - c(X, Y_k) < b_k - b_i$ for all $k \neq i$. Since $\Phi(t_n, X) \rightarrow X$ and $\mathbf{b}^n \rightarrow \mathbf{b}$, it follows that there exists n_0 such that

$$c(\Phi(t_n, X), Y_i) - c(\Phi(t_n, X), Y_k) < b_k^n - b_i^n \quad \forall k \neq i$$

for all $n \geq n_0$. That is, $\Phi(t_n, X) \in \text{Lag}_{ij}(\mathbf{b}^n)$ for all $n \geq n_0$. Now $X \in L_n$ iff $X = \Phi(-t_n, Y)$ for some $Y \in \text{Lag}_{ij}(\mathbf{b}^n)$. But $\Phi(t_n, X) = \Phi(t_n, \Phi(-t_n, Y)) = \Phi(t_n + (-t_n), Y) = \Phi(0, Y) = Y$ from the semigroup property of the flow. Therefore $X \in L_n$ iff $\Phi(t_n, X) \in \text{Lag}_{ij}(\mathbf{b}^n)$, and the claim is then proved.

To complete the analysis we show that the set S in (3.8) has measure zero. Indeed, recall that the target T is contained in the plane $x_3 = \beta$ and Ω is contained in the plane $x_3 = \alpha$ with $\alpha < \beta$. We claim that the set of points X with $x_3 = \alpha$ satisfying

$$\begin{cases} c(X, Y_0) - c(X, Y_1) = t_1 \\ c(X, Y_0) - c(X, Y_2) = t_2 \end{cases} \quad (3.10)$$

is a discrete set for any Y_0, Y_1, Y_2 distinct points in $x_3 = \beta$ and for all $t_1, t_2 \in \mathbb{R}$. In our case (3.10) reads

$$\begin{cases} |X - Y_0| - |X - Y_1| = t_1 \\ |X - Y_0| - |X - Y_2| = t_2 \end{cases}$$

Each of these equations describe a hyperboloid of two sheets, one with foci Y_0, Y_1 , and the other with foci Y_0, Y_2 . These two hyperboloids are intersected with the plane $x_3 = \alpha$ where X lies. Since hyperboloids are quadric surfaces, their intersection with the plane $x_3 = \alpha$ are conics. Now, two conics in the plane intersect in a finite number of points unless they are equal. But if they are equal, then the foci Y_1 and Y_2 must be the equal which is impossible. This shows that the first set in the union (3.8) has measure zero. Finally we note that from (3.6) and using that $\partial\Omega$ is a polygon, the intersection $\partial\Omega \cap H_{ij}(\mathbf{b})$ is finite. This implies that the second set $\text{Lag}_{ij}(\mathbf{b}) \cap \partial\Omega$ also has measure zero. ■

3.2. Monotonicity of the map G

Denote $DG(\mathbf{b})$ the Jacobian matrix of G at a point $\mathbf{b} \in \mathbb{R}^N$. By invariance of the Laguerre cells under addition of a constant, the one-dimensional space $\mathbb{R}\mathbf{e}$, with $\mathbf{e} = (1, 1, \dots, 1)$, is always included in $\ker(DG(\mathbf{b}))$. The next theorem proves the converse inclusion, i.e. $\ker(DG(\mathbf{b})) = \mathbb{R}\mathbf{e}$, whenever all the Laguerre cells have positive mass, i.e. $G_i(\mathbf{b}) > 0$ for all $i \in \{1, \dots, N\}$. This implies a strong monotonicity of the refracted distribution map G , which is used to prove convergence of a damped Newton algorithm in the next section.

Theorem 3.5. *Assume that the conditions of Theorem 3.2 hold, that $\rho \geq 0$, and that*

$$\mathbf{Z} = \text{Int}(\Omega) \cap \{X \in \Omega : \rho(X) > 0\}$$

is a connected set. Let G be the mapping given in (3.2), let

$$S_+ = \{\mathbf{b} = (b_1, \dots, b_N) : G_i(\mathbf{b}) > 0 \quad \forall 1 \leq i \leq N\},$$

and set $\mathbf{e} = (1, 1, \dots, 1)$. Then for each $\mathbf{b} \in S_+$ the matrix $DG(\mathbf{b})$ is symmetric negative semi-definite and $\ker(DG(\mathbf{b})) = \mathbb{R}\mathbf{e}$.

Definition 3.6. The $N \times N$ matrix H is reducible if there exist non empty sets A, B with $A \cap B = \emptyset$, $A \cup B = \{1, \dots, N\}$ such that $H_{\alpha\beta} = 0$ for $\alpha \in A$ and $\beta \in B$. The matrix H is irreducible if it is not reducible.

Lemma 3.7. *Let $H = (H_{ij})_{1 \leq i, j \leq N}$ be an $N \times N$ symmetric matrix satisfying $H_{i,j} \geq 0$ for $i \neq j$ and*

$$H_{ii} = - \sum_{j \neq i} H_{ij} \quad 1 \leq i \leq N. \quad (3.11)$$

Then H is negative semidefinite. If in addition H is irreducible, then $\ker(H) = \mathbb{R}\mathbf{e}$.

Proof of Theorem 3.5. Here we apply the previous Lemma to $H = DG(\mathbf{b})$. From (3.5), (3.11) holds, and from (3.4), $G_{ij}(\mathbf{b}) \geq 0$ for any $j \neq i$. To prove the theorem, by Lemma 3.7 it suffices to prove that the matrix $DG(\mathbf{b}) := (G_{ij}(\mathbf{b}))_{i,j}$ is irreducible for $\mathbf{b} \in S_+$. We proceed in steps.

Step 1. If

$$S = \bigcup_{Y_i \neq Y_j \neq Y_k} \text{Lag}_{ijk}(\mathbf{b}),$$

then $\mathbf{Z} \setminus S$ is open and path-connected. Indeed, by the proof of Theorem 3.2, we know that the set S has zero length, or more precisely zero one-dimensional Hausdorff measure. By [13, Lemma 49], the fact that \mathbf{Z} is path-connected implies that $\mathbf{Z} \setminus S$ is path-connected.

Step 2. For each $1 \leq i \leq N$, $\text{Lag}_i(\mathbf{b}) \cap (\mathbf{Z} \setminus S) \neq \emptyset$.

Since $\mathbf{b} \in S_+$, $\rho(\text{Lag}_i(\mathbf{b})) := \int_{\text{Lag}_i(\mathbf{b})} \rho(X) dX > 0$. Since S is negligible,

$$\rho(\text{Lag}_i(\mathbf{b}) \cap (\mathbf{Z} \setminus S)) = \rho(\text{Lag}_i(\mathbf{b}) \cap \mathbf{Z}) = \rho(\text{Lag}_i(\mathbf{b})),$$

where we used the definition of \mathbf{Z} and the assumption $\rho(\partial\Omega) = 0$ to get the last equality. Since by assumption $\rho(\text{Lag}_i(\mathbf{b})) > 0$, we directly get that $\text{Lag}_i(\mathbf{b}) \cap (\mathbf{Z} \setminus S)$ is nonempty.

Step 3. Let $i \neq j$. If $X \in (\mathbf{Z} \setminus S) \cap \text{Lag}_i(\mathbf{b}) \cap \text{Lag}_j(\mathbf{b})$, then $G_{ij}(\mathbf{b}) > 0$.

Indeed, since $X \in S^c$,

$$\begin{aligned} c(X, Y_i) + b_i &= c(X, Y_j) + b_j \\ c(X, Y_i) + b_i &< c(X, Y_k) + b_k \quad \forall k \neq i, j. \end{aligned}$$

Then by continuity of c and ρ there exists a ball $B_r(X)$ such that

$$c(X', Y_i) + b_i < c(X', Y_k) + b_k \quad \forall X' \in B_r(X) \quad \forall k \neq i, j,$$

and with

$$\rho(X') > 0 \quad \forall X' \in B_r(X).$$

This implies that

$$\{X' : c(X', Y_i) + b_i = c(X', Y_j) + b_j\} \cap B_r(X) \subset \text{Lag}_i(\mathbf{b}) \cap \text{Lag}_j(\mathbf{b}) = \text{Lag}_{ij}(\mathbf{b}).$$

As shown in the proof of Theorem 3.2, the set $\{X' : c(X', Y_i) + b_i = c(X', Y_j) + b_j\}$ is a conic and in particular a 1-dimensional manifold. Therefore

$$\begin{aligned} G_{ij}(\mathbf{b}) &= \int_{\text{Lag}_{ij}(\mathbf{b})} \frac{\rho(X')}{|\nabla_X c(X', Y_i) - \nabla_X c(X', Y_j)|} dX' \\ &\geq \int_{\{X' : c(X', Y_i) + b_i = c(X', Y_j) + b_j\} \cap B_r(X)} \frac{\rho(X')}{|\nabla_X c(X', Y_i) - \nabla_X c(X', Y_j)|} dX' > 0. \end{aligned}$$

To conclude the proof of the irreducibility of DG , we suppose by contradiction that there exists $\mathbf{b} \in S_+$ such that the matrix $DG(\mathbf{b})$ is reducible. This means there exist non empty disjoint sets I and J such that $\{1, \dots, N\} = I \cup J$ with $G_{ij}(\mathbf{b}) = 0$ for all $(i, j) \in I \times J$. Let

$$Z_I = \bigcup_{i \in I} \text{Lag}_i(\mathbf{b}) \cap (\mathbf{Z} \setminus S), \quad Z_J = \bigcup_{i \in J} \text{Lag}_i(\mathbf{b}) \cap (\mathbf{Z} \setminus S).$$

Then from Steps 2 and 3, the sets Z_I and Z_J are non empty and disjoint. Since $\bigcup_{1 \leq i \leq N} \text{Lag}_i(\mathbf{b}) = \Omega$ and $\text{Lag}_i(\mathbf{b})$ are closed in Ω , we have that $\text{Lag}_i(\mathbf{b}) \cap (\mathbf{Z} \setminus S)$ are relatively closed subsets of $\mathbf{Z} \setminus S$ with $\mathbf{Z} \setminus S = Z_I \cup Z_J$ contradicting the connectedness of $\mathbf{Z} \setminus S$. \blacksquare

4. Implementation and numerical experiments

4.1. Damped Newton algorithm

As shown in the previous section, solving the near-field metasurface refractor problem with target $\mu = \sum_{1 \leq i \leq N} g_i \delta_{Y_i}$ amounts to solve the non-linear system $G(\mathbf{b}) = \mathbf{g}$ (see (3.3)) with $\mathbf{g} = (g_1, \dots, g_N)$. We use below the damped Newton algorithm introduced in [11] to solve this equation. To do so, we pick an initialization vector \mathbf{b}^0 (see Remark 4.5) such that all Laguerre cells have a positive amount of mass, and we denote

$$\varepsilon = \frac{1}{2} \min \left\{ \min_{1 \leq i \leq N} G_i(\mathbf{b}^0), \min_{1 \leq i \leq N} g_i \right\} > 0$$

Adding a constant to \mathbf{b}^0 if necessary, we may assume that $b^0 \in \{\mathbf{e}\}^\perp$ where $\mathbf{e} = (1, \dots, 1)$. Thus, \mathbf{b}^0 belongs to the set

$$S = \left\{ \mathbf{b} \in \mathbb{R}^N : \forall i \in \{1, \dots, N\} G_i(\mathbf{b}) \geq \varepsilon \right\} \cap \{\mathbf{e}\}^\perp.$$

4.1.1. Algorithm

Given an iterate \mathbf{b}^k , we explain how to define the next iterate \mathbf{b}^{k+1} . We first denote \mathbf{v}^k the solution to the system

$$\begin{cases} DG(\mathbf{b}) \mathbf{v}^k = \mathbf{g} - G(\mathbf{b}) \\ \sum_{i=1}^N v_i^k = 1, \end{cases} \quad (4.1)$$

which exists and is unique by Theorem 3.5. Denoting $\mathbf{b}_\tau^k = \mathbf{b}^k + \tau \mathbf{v}^k$, we introduce

$$E^k = \left\{ 2^{-\ell} : \ell \in \mathbb{N}, \mathbf{b}_{2^{-\ell}}^k \in S, \left| G(\mathbf{b}_{2^{-\ell}}^k) - \mathbf{g} \right| \leq \left(1 - \frac{2^{-\ell}}{2} \right) |G(\mathbf{b}^k) - \mathbf{g}| \right\}$$

$$\tau^k = \max E^k.$$

We then denote

$$\mathbf{b}^{k+1} = \mathbf{b}^k + \tau^k \mathbf{v}^k.$$

Proposition 4.1 (Linear convergence). *Under the assumptions of Theorems 3.2 and 3.5, there exists a constant $\tau^* \in (0, 1)$ such that*

$$|G(\mathbf{b}^k) - \mathbf{g}| \leq \left(1 - \frac{\tau^*}{2} \right)^k |G(\mathbf{b}^0) - \mathbf{g}|$$

Proof. Thanks to Theorems 3.2 and 3.5, the refracted distribution G satisfies the assumptions of [13, Prop. 50], which implies the result. \blacksquare

4.2. Computation of Laguerre cells

Computing the Laguerre cells associated to the near-field refractor metasurface problem is not an easy task, because these cells have curved boundaries (see Figure 4.1), are not convex, etc. In this section, we show that the Laguerre cells can be obtained by using power diagrams. The advantage of this formulation is that there are very efficient algorithms and software libraries available to construct 3D power diagrams, with near-linear complexity in N for non-degenerate input.

Definition 4.2. Let $Q = \{(q_i, \omega_i)\}_{1 \leq i \leq N}$ be a weighted cloud point set, i.e., $q_i \in \mathbb{R}^3$ and $\omega_i \in \mathbb{R}$. Then for each $1 \leq i \leq N$, the i -th power diagram of Q is defined by

$$\text{Pow}_i(Q) = \left\{ x \in \mathbb{R}^3 : |x - q_i|^2 + \omega_i \leq |x - q_j|^2 + \omega_j \quad \forall j \in \{1, \dots, N\} \right\}.$$

Let us define

$$H_i(\mathbf{b}) = \left\{ X \in \mathbb{R}^2 \times \{\alpha\} : |X - Y_i| + b_i \leq |X - Y_j| + b_j, \quad \forall 1 \leq j \leq N \right\}, \quad 1 \leq i \leq N,$$

with $\mathbf{b} = (b_1, \dots, b_N)$, $0 < \alpha < \beta$, and the points $Y_i = (y_i, \beta)$ lie in the horizontal plane $\mathbb{R}^2 \times \{\beta\}$. From the definition of Laguerre cell in (3.1), we have

$$\text{Lag}_i(\mathbf{b}) = H_i(\mathbf{b}) \cap \Omega.$$

Proposition 4.3 (Point Source/Near-Field). *We assume the following condition*

$$\forall i, j \in \{1, \dots, N\} \quad |b_i - b_j| < \sqrt{4(\alpha - \beta)^2 + |y_i - y_j|^2}. \quad (4.2)$$

Then, for each $i \in \{1, \dots, N\}$, one has

$$H_i(\mathbf{b}) = P_{\mathbb{R}^2 \times \{\alpha\}} \left(\text{Pow}_i(Q) \cap \Sigma_i^+ \right)$$

where $P_{\mathbb{R}^2 \times \{\alpha\}}$ denotes the orthogonal projection onto $\mathbb{R}^2 \times \{\alpha\}$, $Q = \{(q_i, \omega_i)\}_{i=1}^N$ is the weighted point cloud with $q_i = (y_i, -b_i)$ and $\omega_i = -2b_i^2$, and where Σ_i^+ is one sheet of a hyperboloid given by $\Sigma_i^+ = \{(x, |X - Y_i| + b_i) : X = (x, \alpha), x \in \mathbb{R}^2\}$. Therefore,

$$\text{Lag}_i(\mathbf{b}) = P_{\mathbb{R}^2 \times \{\alpha\}} \left(\text{Pow}_i(Q) \cap \Sigma_i^+ \right) \cap \Omega.$$

In practice, condition (4.2) is not restrictive because to use the damped Newton algorithm from Section 4.1, one needs to assume that the Laguerre cells at the initialization vector \mathbf{b}^0 are non empty which by the corollary below implies (4.2).

Corollary 4.4. *If the vector \mathbf{b} satisfies $\text{Lag}_i(\mathbf{b}) \neq \emptyset$ for each $1 \leq i \leq N$, then*

$$\text{Lag}_i(\mathbf{b}) = P_{\mathbb{R}^2 \times \{\alpha\}} \left(\text{Pow}_i(Q) \cap \Sigma_i^+ \right) \cap \Omega,$$

for all $1 \leq i \leq N$.

Proof. Fix $1 \leq i, j \leq N$ with $i \neq j$ and suppose that $\mathbf{b} = (b_1, \dots, b_N)$ is such that $\text{Lag}_i(\mathbf{b}) \neq \emptyset$ and $\text{Lag}_j(\mathbf{b}) \neq \emptyset$ contain points X_i and X_j respectively. Then,

$$|X_i| + |X_i - Y_i| = c(X_i, Y_i) + b_i \leq c(X_i, Y_j) + b_j = |X_i| + |X_i - Y_j| + b_j.$$

Thus, $b_i - b_j \leq |Y_i - Y_j| = |y_i - y_j|$. By symmetry, we get

$$|b_i - b_j| \leq |y_i - y_j| < \sqrt{4(\alpha - \beta)^2 + |y_i - y_j|^2}. \quad \blacksquare$$

Remark 4.5. If $\alpha = \beta$, then the Laguerre diagram is known as *Apollonius diagram* where all the surfaces Σ_i^+ are half-cones. When $\alpha \neq \beta$, then each Σ_i^+ is not anymore a cone but a sheet of a hyperboloid.

Remark 4.6 (Initialization). To apply the algorithm from Section 4.1, we need to find an initial vector $\mathbf{b}^0 = (b_1, \dots, b_N)$ for which the corresponding Laguerre cells are not empty. Taking $\mathbf{b}^0 = 0$ this is the case when

$$P_{\mathbb{R}^2 \times \{\alpha\}}(Y_i) \in \Omega, \quad \forall i \in \{1, \dots, N\}.$$

Indeed, if we denote by $X_i = (y_i, \alpha)$ such a point, we see that $|X_i - Y_i| = |\beta - \alpha| \leq |X_i - Y_j|$ for any j , implying that $X_i \in \text{Lag}_i(0)$. For other options to choose the initialization vector see [14, Section 2.3].

4.3. Proof of Proposition 4.3

Let us consider the hyperboloid of two sheets

$$\Sigma_i = \left\{ (x, x_3) : |X - Y_i|^2 = (x_3 - b_i)^2, X = (x, \alpha), x \in \mathbb{R}^2 \right\}$$

with $Y_i = (y_i, \beta)$, $\beta > \alpha$. The upper sheet of this hyperboloid is given parametrically by

$$\Sigma_i^+ = \left\{ (x, |X - Y_i| + b_i) : X = (x, \alpha), x \in \mathbb{R}^2 \right\}$$

and the lower sheet is given by

$$\Sigma_i^- = \left\{ (x, -|X - Y_i| + b_i) : X = (x, \alpha), x \in \mathbb{R}^2 \right\}.$$

Clearly, Σ_i^- and Σ_i^+ are symmetric with respect to the hyperplane $\{x_3 = b_i\}$, and $\Sigma_i = \Sigma_i^- \cup \Sigma_i^+$.

We first need to determine the relative positions of the hyperboloids Σ_i and Σ_j .

Lemma 4.7. *We have the following:*

- (1) *If $\Sigma_i^+ \cap \Sigma_j^- = \emptyset$, then Σ_i^+ is strictly above Σ_j^- , i.e., for any $x \in \mathbb{R}^2$ such that $(x, x_3^i) \in \Sigma_i^+$ and $(x, x_3^j) \in \Sigma_j^-$, one has $x_3^i > x_3^j$.*
- (2) *$\sqrt{4(\alpha - \beta)^2 + |y_i - y_j|^2} > b_j - b_i$ if and only if $\Sigma_i^+ \cap \Sigma_j^- = \emptyset$.*
- (3) *If $\Sigma_i^+ \cap \Sigma_j^- \neq \emptyset$, then Σ_i^+ is strictly below Σ_j^+ , i.e., for any $x \in \mathbb{R}^2$ such that $(x, x_3^i) \in \Sigma_i^+$ and $(x, x_3^j) \in \Sigma_j^+$, one has $x_3^i < x_3^j$.*

Proof. (1). Since Σ_i^+ opens upwards and Σ_j^- opens downwards, if they don't intersect, it is clear that Σ_i^+ must be strictly above Σ_j^- .

(2). We have $\Sigma_i^+ \cap \Sigma_j^- \neq \emptyset$ iff there exists $X \in \mathbb{R}^2 \times \{\alpha\}$ with

$$|X - Y_i| + |Y_j - X| = b_j - b_i.$$

On the other hand, for each $X \in \mathbb{R}^2 \times \{\alpha\}$, one has

$$|X - Y_i| + |Y_j - X| \geq |X_{i,j} - Y_i| + |X_{i,j} - Y_j| = 2\sqrt{(\alpha - \beta)^2 + |y_i - y_j|^2}/4,$$

where $X_{i,j} = ((y_i + y_j)/2, \alpha)$. Therefore, $\sqrt{4(\alpha - \beta)^2 + |y_i - y_j|^2} > b_j - b_i$ implies $\Sigma_i^+ \cap \Sigma_j^- = \emptyset$.

Vice versa, from Item (1), $|X - Y_i| + b_i > -|X - Y_j| + b_j$ for each $X = (x, \alpha)$ and so $b_j - b_i$ satisfies the desired inequality.

(3). By contradiction. Suppose there are points $(x, x_3^i) \in \Sigma_i^+$ and $(x, x_3^j) \in \Sigma_j^+$ with $x_3^i \geq x_3^j$. If $X = (x, \alpha)$, then $|X - Y_i| + b_i = x_3^i \geq x_3^j = |X - Y_j| + b_j$, and so $b_j - b_i \leq |Y_i - Y_j|$ from triangle inequality. Now, $\sqrt{4(\alpha - \beta)^2 + |y_i - y_j|^2} \leq b_j - b_i$ from (2). Since $|Y_i - Y_j| < \sqrt{4(\alpha - \beta)^2 + |y_i - y_j|^2}$, we obtain a contradiction. \blacksquare

The previous lemma leads to the following.

Lemma 4.8. Fix i, j and define the sets

$$L_{i,j}^{\leq} := \left\{ X \in \mathbb{R}^2 \times \{\alpha\} : |X - Y_i| + b_i \leq |X - Y_j| + b_j \right\} \supset \text{Lag}_i(\mathbf{b}),$$

$$H_{ij}^{\leq} := \left\{ x \in \mathbb{R}^3 : |x - q_i|^2 + \omega_i \leq |x - q_j|^2 + \omega_j \right\}, \quad \omega_j = -2b_j^2; \quad q_j = (y_j, -b_j).$$

We have:

(1) If $\sqrt{4(\alpha - \beta)^2 + |y_i - y_j|^2} > b_j - b_i$, then

$$L_{i,j}^{\leq} = \text{P}_{\mathbb{R}^2 \times \{\alpha\}} \left(H_{ij}^{\leq} \cap \Sigma_i^+ \right)$$

(2) If $\sqrt{4(\alpha - \beta)^2 + |y_i - y_j|^2} \leq b_j - b_i$, then $L_{i,j}^{\leq} = \mathbb{R}^2 \times \{\alpha\}$.

Proof. (1). Let $X = (x, \alpha) \in L_{i,j}^{\leq}$, and $x_3 = |X - Y_i| + b_i$. By Lemma 4.7 (2) and (1), the point $(x, x_3) \in \Sigma_i^+$ is above Σ_j^- , and so $x_3 - b_j > -|Y_j - X|$. By definition of $L_{i,j}^{\leq}$, we also have $x_3 - b_j \leq |Y_j - X|$, which implies

$$(x_3 - b_i)^2 = |X - Y_i|^2 \quad \text{and} \quad (x_3 - b_j)^2 \leq |X - Y_j|^2.$$

Expanding these two equations, one gets

$$\begin{cases} x_3^2 - 2b_i x_3 + b_i^2 = |X|^2 - 2X \cdot Y_i + |Y_i|^2 \\ x_3^2 - 2b_j x_3 + b_j^2 \leq |X|^2 - 2X \cdot Y_j + |Y_j|^2. \end{cases}$$

Subtracting the first line from the second line yields

$$-2(x, x_3) \cdot (y_i, -b_i) + |Y_i|^2 - b_i^2 \leq -2(x, x_3) \cdot (y_j, -b_j) + |Y_j|^2 - b_j^2$$

which can be rewritten as

$$|(x, x_3) - (y_i, -b_i)|^2 - 2b_i^2 \leq |(x, x_3) - (y_j, -b_j)|^2 - 2b_j^2.$$

This means $(x, x_3) \in H_{ij}^{\leq}$ and so $(x, x_3) \in H_{ij}^{\leq} \cap \Sigma_i^+$. To show the opposite inclusion, let $(x, x_3) \in H_{ij}^{\leq} \cap \Sigma_i^+$ and put $X = (x, \alpha)$. Then one has

$$\begin{cases} x_3 = |X - Y_i| + b_i \\ |(x, x_3) - (y_i, -b_i)|^2 - 2b_i^2 \leq |(x, x_3) - (y_j, -b_j)|^2 - 2b_j^2. \end{cases}$$

Reversing the previous calculation, one gets $(x_3 - b_j)^2 \leq |X - Y_j|^2$. This obviously implies $-|X - Y_j| \leq x_3 - b_j \leq |X - Y_j|$, which gives in particular that $X \in L_{i,j}^{\leq}$, completing the proof of (1).

(2). From Lemma 4.7 (2), $\Sigma_i^+ \cap \Sigma_j^- \neq \emptyset$ and so from Item (3) in that lemma, Σ_i^+ is strictly below Σ_j^+ . That is, $b_i + |X - Y_i| < b_j + |X - Y_j|$ for all $x \in \mathbb{R}^2$, $X = (x, \alpha)$. This means $L_{i,j}^{\leq}$ is the whole plane $\mathbb{R}^2 \times \{\alpha\}$. ■

Proof of Proposition 4.3. Let $i \in \{1, \dots, N\}$. From (4.2) we can apply Lemma 4.8(1) to obtain

$$H_i(\mathbf{b}) = \bigcap_{1 \leq j \leq N} L_{i,j}^{\leq} = \bigcap_{1 \leq j \leq N} \text{P}_{\mathbb{R}^2 \times \{\alpha\}} \left(H_{ij}^{\leq} \cap \Sigma_i^+ \right) = \text{P}_{\mathbb{R}^2 \times \{\alpha\}} \left(\Sigma_i^+ \cap \bigcap_{1 \leq j \leq N} H_{ij}^{\leq} \right)$$

Since by definition $\text{Pow}_i(Q) = \bigcap_{1 \leq j \leq N} H_{ij}^{\leq}$, the proposition follows. ■

4.4. Numerical experiments

In all three numerical experiments, we assume that the source measure $\rho \equiv \frac{1}{4}$ is uniform over the square $\Omega = [-1, 1]^2 \times \{\alpha\}$, and we also assume that the metasurface is at height $\alpha = 1$. The Laguerre

cells are computed using Proposition 4.3, by intersecting 3D power cells with a quadric. To describe the algorithm, we use the notation from that proposition:

- First, we compute 3D the power diagram $(\text{Pow}_i(Q))_{1 \leq i \leq N}$ using the CGAL library and we restrict each cell to the lifted domain $\Omega \times \mathbb{R}$ by computing the intersection $P_i = \text{Pow}_i(Q) \cap (\Omega \times \mathbb{R})$. In the implementation, we assume that $\Omega \subseteq \mathbb{R}^2$ is a convex polygon.
- For every pair $i \neq j \in \{1, \dots, N\}$, we compute the curve γ_{ij} corresponding to the projection on $\mathbb{R}^2 \times \{\alpha\}$ of the facet $P_i \cap P_j$ with the quadric Σ_i^+ ,

$$\gamma_{ij} = \text{P}_{\mathbb{R}^2 \times \{\alpha\}}(P_i \cap P_j \cap \Sigma_i^+).$$

In practice, we need to make this computation only if the power cells already have a non-empty interface, i.e. if $P_i \cap P_j \neq \emptyset$. We also note that by Proposition 4.3,

$$\text{Lag}_i(\mathbf{b}) \cap \text{Lag}_j(\mathbf{b}) = \gamma_{ij}.$$

- We finally compute the intersection of each Laguerre cell with the boundary of the domain using the formula

$$\gamma_{i,\infty} = \text{Lag}_i(\mathbf{b}) \cap \partial\Omega = \text{P}_{\mathbb{R}^2 \times \{\alpha\}}(\text{Pow}_i(Q)) \cap \partial\Omega.$$

By construction, the boundary of the i th Laguerre cell is given by

$$\partial \text{Lag}_i(\mathbf{b}) = \gamma_{i,\infty} \cup \bigcup_{j \neq i} \gamma_{ij},$$

and the union is disjoint up to a finite set, which is negligible. We may then use this description of the boundary of the cell $\text{Lag}_i(\mathbf{b})$ to compute the integral of ρ over $\text{Lag}_i(\mathbf{b})$ using divergence theorem

$$G_i(\mathbf{b}) = \int_{\text{Lag}_i(\mathbf{b})} \rho(X) dX = \frac{1}{8} \int_{\partial \text{Lag}_i(\mathbf{b})} X \cdot n_i(X) dX,$$

where n_i denotes the exterior normal to $\text{Lag}_i(\mathbf{b})$, and where the second integral is 1-D. The partial derivatives are computed using (3.4): for $i \neq j$ we have

$$\frac{\partial G_i}{\partial b_j}(\mathbf{b}) = \int_{\gamma_{ij}} \frac{1}{4} \frac{1}{|\nabla_X c(X, Y_i) - \nabla_X c(X, Y_j)|} dX,$$

where again the integrals are one dimensional. The code to compute the intersection between the power cell $\text{Pow}_i(Q)$ and the quadric Σ_i^+ and to perform the numerical integration is written in a combination of C++ and Python, and is available online³, as well as the experiments presented below.

4.4.1. Effect of changes in $\beta - \alpha$ on the shape of $\text{Lag}_i(\mathbf{b})$

In the first numerical experiment, we study the effect of the distance between the metasurface and the target, $\delta = \beta - \alpha$, on the shape of the Laguerre cells. We assume that the target is of the form

$$\nu = \frac{1}{N} \sum_{1 \leq i \leq 25} \delta_{y_i},$$

where $N = 25$ and $\{y_1, \dots, y_N\}$ is a uniform 5×5 grid contained in the square $[0, 1]^2$, and we solve the optimal transport problem between ρ and ν . Our goal in this first experiment is to visualize the effect of changes in δ , the vertical distance between the source and the metasurface, on the shape of the

³<https://github.com/mrgt/ot-optics>

solution. We initialize the damped Newton algorithm described in Section 4.1 with $\mathbf{b}^0 = (0, \dots, 0)$. The associated Laguerre cells coincides with the Voronoi cells of the point cloud $\{Y_1, \dots, Y_N\}$, i.e.

$$\text{Vor}_i = \{X \in \mathbb{R}^2 \times \{\alpha\} \mid \forall j \in \{1, \dots, N\}, |X - Y_i| \leq |X - Y_j|\}.$$

and is shown on the first row and column of Figure 4.1. We solve the near-field metasurface problem for several values of δ , and we display the Laguerre cells of the solution. In particular, one can see that for $\delta = 2$, the solution is very similar to the solution of the optimal transport problem for the “standard” quadratic cost. Indeed, as detailed below in Lemma 5.5, when the target T tends to infinity, the phases for Near Field problem converge to phases for Far Field problem, that correspond to an optimal transport problem for the cost $c(X, Y) = -X \cdot Y$, or equivalently for the quadratic cost.

4.4.2. Convergence speed

In our second numerical experiment, the target measure ν approximates the restriction of the Gaussian $e^{-2|y|^2}$ to the unit square $[-1, 1]^2 \times \{\alpha\}$. More precisely, the measure ν is of the form

$$\nu = \frac{1}{N} \sum_{1 \leq i \leq N} \nu_i \delta_{y_i},$$

where $N = n^2$ and $n \in \{5, 10, 20, 30, 40, 50, 100\}$. The points $\{y_1, \dots, y_N\}$ form a uniform $n \times n$ grid in the square $[-1, 1]^2 \times \{\alpha\}$. The mass ν_i of the Dirac δ_{y_i} is defined by evaluating a Gaussian at y_i :

$$\nu_i = e^{-2|y_i|^2} / \sum_{1 \leq j \leq N} e^{-2|y_j|^2}.$$

Figure 4.3 displays the solution of this problem for $N = 100^2$. Figure 4.2 displays the decrease of the numerical error along the iterations of the algorithm, defined as

$$\varepsilon_k = \left(\sum_i (H_i(\mathbf{b}^k) - \nu_i)^2 \right)^{1/2},$$

for several values of N . One observes a linear convergence for the first iterations, followed after only 4 iterations by a quadratic convergence. Proposition 4.1 does not explain this quadratic convergence, but such a quadratic convergence has been established in other similar contexts [11]. In particular, one can see from this figure that the number of iterations in the Damped Newton algorithm is particularly low: a numerical error of 10^{-8} is reached in less than 8 iterations, even for $N = 10^4$.

4.4.3. Visualization of the phase

In this last numerical experiment, the target is uniform over four discretized disks (Figure 4.4, top row) or over a discretized letter H (Figure 4.4, bottom row), i.e. $\nu \equiv 4/N$ where N is the number of points composing the discretized shapes. Figure 4.4 displays the Laguerre cells corresponding to the solution of the near-field metasurface problem. We also display the corresponding phase discontinuity ϕ , which can be computed thanks to Theorem 2.3. On the “four disks” example, one may notice that the gradient of the phase discontinuity ϕ seems to exhibit a discontinuity on the “cross” $\{0\} \times [0, 1] \times \{\alpha\} \cup [0, 1] \times \{0\} \times \{\alpha\}$: this corresponds to a jump in the transport map which is necessary to cross the void between the four disks.

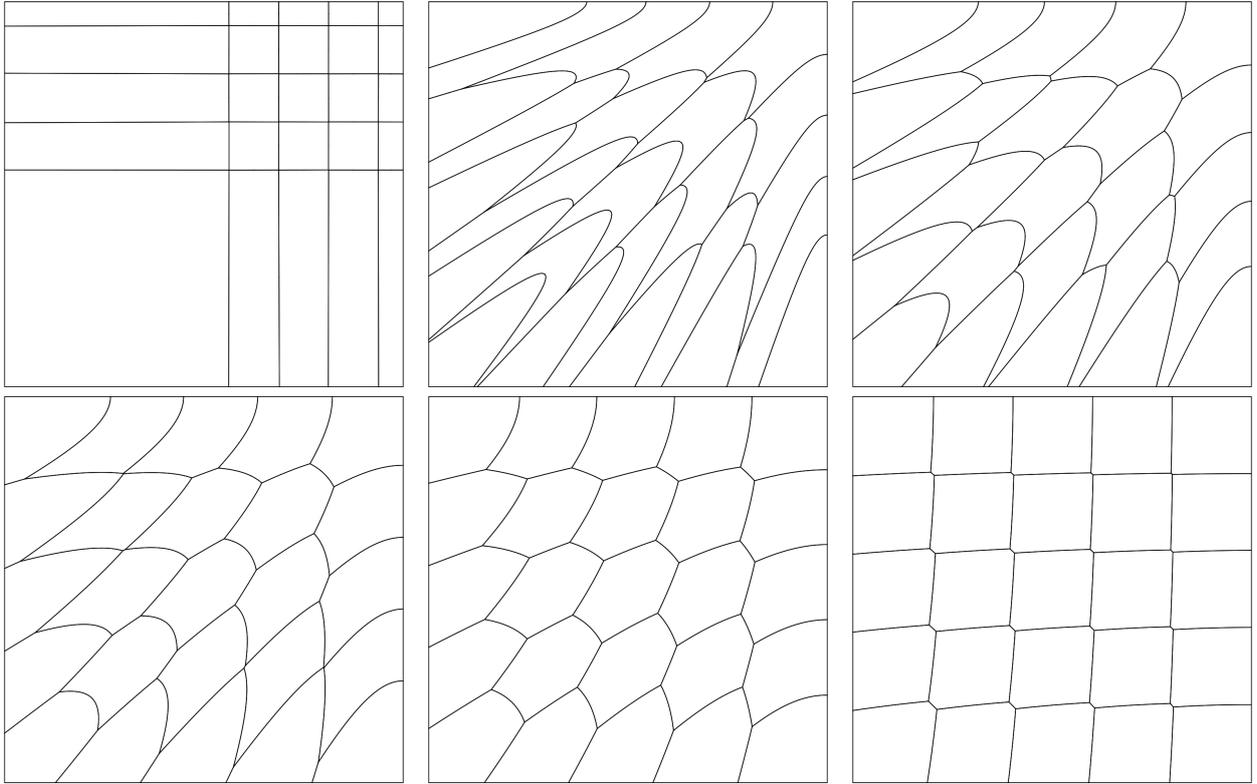


FIGURE 4.1. From left to right and top to bottom: The first image displays the Voronoi cells of $\{Y_1, \dots, Y_N\}$. Then, each image displays the Laguerre cells associated to the solutions of the near-field metasurface problem described in Section 4.4.1 for $\delta \in \{0.1, 0.2, 0.3, 0.5, 2\}$.

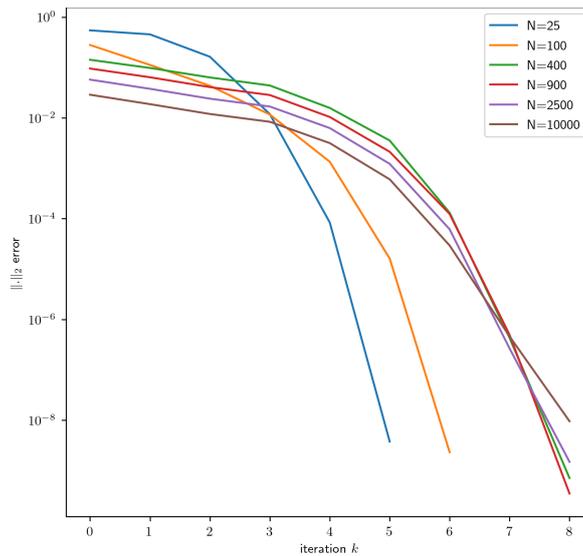


FIGURE 4.2. Convergence of the numerical error in terms of the iteration number for the near-field metasurface problem described in Section 4.4.2, for $N \in \{5, 10, 20, 30, 40, 50, 100\}^2$.

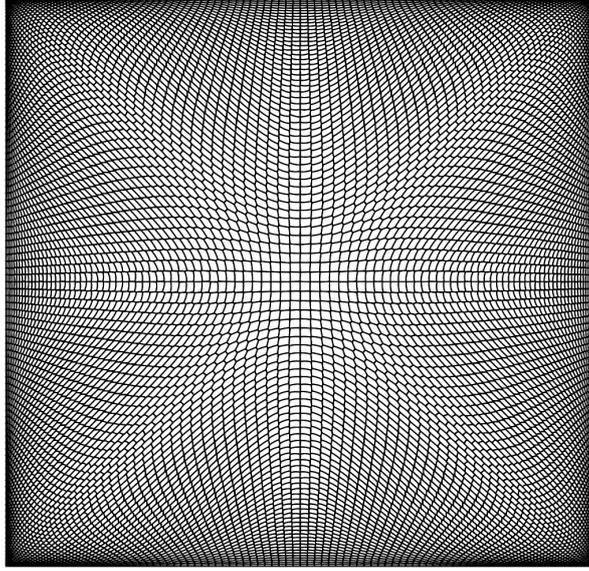


FIGURE 4.3. Laguerre diagram associated to the solution of the near-field metasurface problem described in Section 4.4.2, for $N = 100^2$.

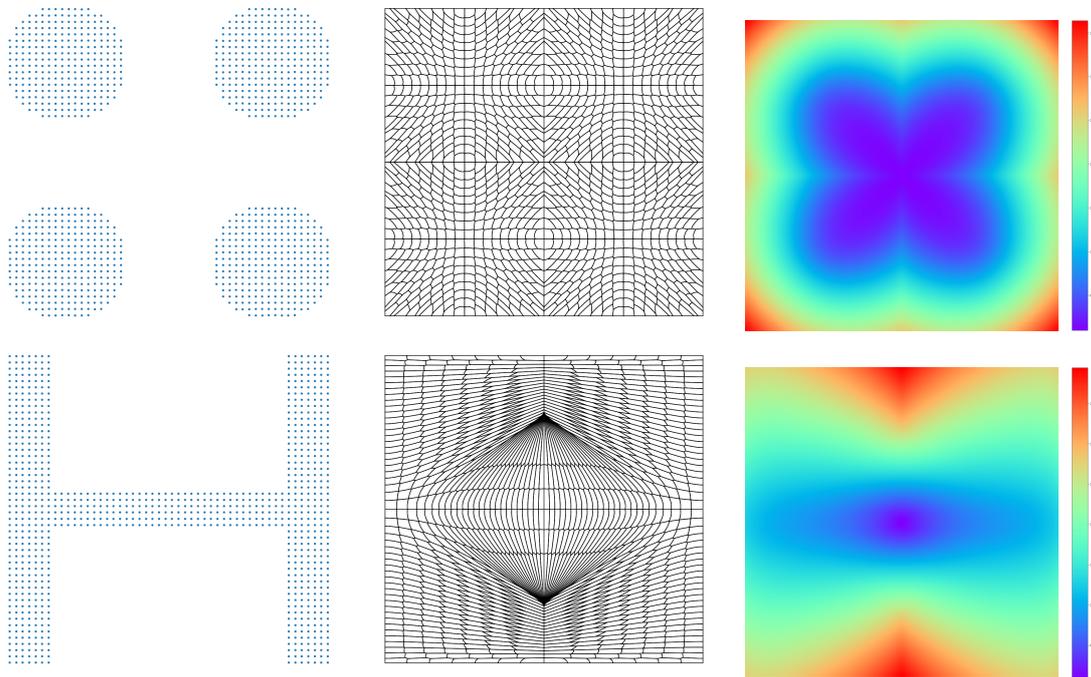


FIGURE 4.4. Near-field metasurface with a target measure supported over four discretized disks (top) or a discretized letter H (bottom): Support of the target measure (left), Laguerre cells associated to the solution (middle), and the corresponding phase discontinuity ϕ (right).

5. Refraction into the far field

We consider here the case when incident rays emanate in a collimated beam and the case when they emanate from a point source. Since the arguments to treat these problems are similar to the ones used in Section 2, we only indicate the modifications that are needed.

5.1. Collimated beam

Let Γ be the horizontal plane $x_3 = a$ in \mathbb{R}^3 , $\mathbf{e} = (0, 0, 1)$. The phase discontinuity function $\phi(x)$ with $x = (x_1, x_2, x_3)$ defined in a neighborhood of Γ such that the metasurface (Γ, ϕ) refracts all vertical rays having direction \mathbf{e} into a fixed unit direction $\mathbf{m} = (m_1, m_2, m_3)$, with $m_3 > 0$, is given by

$$\phi(x) = \mathbf{v} \cdot x, \text{ with } \mathbf{v} = (\mathbf{m} \cdot \mathbf{e}) \mathbf{e} - \mathbf{m} = (-m_1, -m_2, 0);$$

see [10, Theorem 4.1] for a proof in the more general case when \mathbf{m} is a variable set of directions depending on x . Notice that if $\mathbf{m} = (m_1, m_2, m_3)$ and $\mathbf{m}' = (m'_1, m'_2, m'_3)$ are two unit vectors with $m_3, m'_3 > 0$ and $(m_1, m_2) = (m'_1, m'_2)$, then $\mathbf{m} = \mathbf{m}'$.

Each vector $\mathbf{m} = (m_1, m_2, m_3) \in S^2$ with $m_3 > 0$ can be identified with its projection (m_1, m_2) on the disk of radius one around $(0, 0)$ where $m_3 = \sqrt{1 - m_1^2 - m_2^2}$.

Fix a compact region $\Omega \subset \Gamma$ with points $x = (x_1, x_2, a)$ and a compact region $\Omega^* \subset S^2_+$.

Definition 5.1 (Admissible phase). The function $\phi : \Omega \rightarrow \mathbb{R}$ is an admissible phase refracting Ω into Ω^* if for each $x_0 \in \Omega$ there exists $\mathbf{m} \in \Omega^*$ and $b \in \mathbb{R}$ such that

$$\begin{aligned} \phi(x) &\geq b + ((\mathbf{m} \cdot \mathbf{e}) \mathbf{e} - \mathbf{m}) \cdot x := L(\mathbf{m}, b, x), & \forall x \in \Omega, \text{ and} \\ \phi(x_0) &= b + ((\mathbf{m} \cdot \mathbf{e}) \mathbf{e} - \mathbf{m}) \cdot x_0. \end{aligned}$$

We say that $L(\mathbf{m}, b, x)$ is a supporting phase to ϕ at x_0 .

Definition 5.2. Given $x_0 \in \Omega$ and ϕ an admissible phase, we define the set-valued mapping $\mathcal{N}_\phi : \Omega \rightarrow \mathcal{P}(\Omega^*)$ given by

$$\mathcal{N}_\phi(x_0) = \{m \in \Omega^* : \text{there exists } b \in \mathbb{R} \text{ such that } L(\mathbf{m}, b, x) \text{ is a supporting phase to } \phi \text{ at } x_0\};$$

and the inverse map

$$(\mathcal{N}_\phi)^{-1}(m) = \{x \in \Omega : m \in \mathcal{N}_\phi(x)\}.$$

Define the class

$$\mathcal{F} = \{\phi : \Omega \rightarrow \mathbb{R} : \phi \text{ is an admissible phase refracting } \Omega \text{ into } \Omega^*\}.$$

Given $f \in L^1(\Omega)$, non negative, assuming that $\partial\Omega$ has 2-dimensional Lebesgue measure zero, and given a Borel measure μ in Ω^* satisfying $\int_\Omega f(x) dx = \mu(\Omega^*)$, our problem is then to find $\phi \in \mathcal{F}$ solving

$$\mathcal{M}_\phi(E) := \int_{(\mathcal{N}_\phi)^{-1}(E)} f(x) dx = \mu(E) \tag{5.1}$$

for each Borel set $E \subset \Omega^*$. To show existence and uniqueness to this problem, we proceed as in Section 2 with the following changes. The class \mathcal{F} satisfies the following properties that follow immediately from the definitions above

(A1') If $\phi_1, \phi_2 \in \mathcal{F}$, then $\phi_1 \vee \phi_2 = \max\{\phi_1, \phi_2\} \in \mathcal{F}$,

(A2') if $\phi_1(x_0) \geq \phi_2(x_0)$, then $\mathcal{N}_{\phi_1}(x_0) \subset \mathcal{N}_{\phi_1 \vee \phi_2}(x_0)$,

(A3') Given $\mathbf{m} \in \Omega^*$ the functions $L(\mathbf{m}, b, x) \in \mathcal{F}$, $b \in (-\infty, \infty)$, satisfy the following

(a) $\mathbf{m} \in \mathcal{N}_{L(\mathbf{m}, b, x)}(x)$ for all $x \in \Omega$,

- (b) $L(\mathbf{m}, b, x) \leq L(\mathbf{m}, b', x)$ for all $b \leq b'$,
- (c) for each $\mathbf{m} \in \Omega^*$, $L(\mathbf{m}, b, x) \rightarrow +\infty$ uniformly for $x \in \Omega$ as $b \rightarrow +\infty$,
- (d) for each $\mathbf{m} \in \Omega^*$, $\max_{x \in \Omega} |L(\mathbf{m}, b', x) - L(\mathbf{m}, b, x)| \rightarrow 0$ as $b' \rightarrow b$.

Recalling the notation at the beginning of Section 2.3, we now let $\mathcal{X} = \Omega$ and $\mathcal{Y} = \Omega^*$, and with similar arguments but now using conditions (A1')–(A3') instead of (A1), (A2), (A3''), we get that $\mathcal{N}_\phi \in C_s(\Omega, \Omega^*)$ for each $\phi \in \mathcal{F}$. Then to prove existence and uniqueness when $\mu = \sum_{i=1}^N g_i \delta_{\mathbf{m}_i}$, we use [5, Theorem 2.12], for which we only need to verify its hypotheses. In fact, we need to verify that there exist numbers b_1^0, \dots, b_N^0 such that the admissible phase $\phi_0(x) = \max_{1 \leq i \leq N} L(\mathbf{m}_i, b_i^0, x)$, for $x \in \Omega$, satisfies $\mathcal{M}_{\phi_0}(\mathbf{m}_j) \leq g_j$ for $2 \leq j \leq N$. By continuity, given any b_1^0 we can pick b_2^0, \dots, b_N^0 tending to $-\infty$ such that $L(\mathbf{m}_i, b_i^0, x) < L(\mathbf{m}_1, b_1^0, x)$ for all $i \neq 1$ and $x \in \Omega$. Therefore, $\phi_0(x) = L(\mathbf{m}_1, b_1^0, x)$. Since the points $\mathbf{m}_i = (m_1^i, m_2^i, m_3^i) \neq \mathbf{m}_j = (m_1^j, m_2^j, m_3^j)$ for $i \neq j$, the family of planes having equations $z = \alpha - m_1^i x_1 - m_2^i x_2$ are never parallel. Consequently, $t(\mathcal{N}_{\phi_0})^{-1}(\mathbf{m}_i) \subset \partial\Omega$ for $i \neq 1$ and so $\mathcal{M}_{\phi_0}(\mathbf{m}_i) = 0$ for $i \neq 1$. The hypotheses in [5, Theorem 2.12] then hold in our case. In addition, from the conditions (A1')–(A3') above we can apply [5, Theorem 2.12] to obtain the following.

Theorem 5.3. *Let $\mathbf{m}_1, \dots, \mathbf{m}_N$ be distinct points in Ω^* , g_1, \dots, g_N are positive numbers, and $f \in L^1(\Omega)$ with*

$$\int_{\Omega} f(x) dx = \sum_{i=1}^N g_i; \quad (5.2)$$

$\mu = \sum_{i=1}^N g_i \delta_{\mathbf{m}_i}$. Then given any $b_1 \in \mathbb{R}$, there exist numbers b_2, \dots, b_N such that the convex function

$$\phi(x) = \max_{1 \leq i \leq N} \{L(\mathbf{m}_i, b_i, x)\} \quad (5.3)$$

solves (5.1).

Moreover, one can state a convergence result with linear speed, similar to Proposition 4.1, for the Damped Newton algorithm.

5.2. Point source far field

Suppose rays emanate from the origin O , Π is the plane $x_3 = a$ and \mathbf{m} is a unit direction. Then the metasurface (Π, ϕ) refracting rays from O into the direction \mathbf{m} (with $\nabla\phi(x) \cdot e = 0$, $e = (0, 0, 1)$, i.e., ϕ tangential to Π^4) is given by

$$\phi(x) = |x| - \mathbf{m} \cdot x + C \quad (5.4)$$

where $x = (x_1, x_2, x_3)$ and C a constant, see [7, Section 4.A]. Let $\Omega_0, \Omega' \subset S_{\pm}^2$ and let $\Omega = \{\lambda x : x \in \Omega_0, \lambda x \in \Pi\}$.

Definition 5.4 (Admissible phase for the far field). The function $\phi : \Omega \rightarrow \mathbb{R}$ is a far field admissible phase refracting Ω into Ω' if for each $X_0 \in \Omega$ there exists $b \in \mathbb{R}$ and $y \in \Omega'$ such that

$$\phi(X) \geq |X| - y \cdot X + b \quad \forall X \in \Omega, \quad \phi(X_0) = |X_0| - y \cdot X_0 + b.$$

When this happens, we say that $|X| - y \cdot X + b$ supports ϕ at X_0 .

In this case, the analysis about existence and uniqueness of solutions follows the lines already described and therefore we omit more details. It yields a theorem similar to Theorem 5.3 now in terms of the far field supporting phases $|X| - y \cdot X + b$.

We complete the paper mentioning that the phases for near field problem given by Definition 2.1 converge to the phases for far field problem in Definition 5.4 when the target T goes to infinity along fixed directions as indicated in the following lemma.

⁴Each $\phi(x) = |x| - \mathbf{m} \cdot x + h(x_3)$ satisfies (2.1) with $n_1 = n_2 = 1$ but is not tangential to Π unless h is constant.

Lemma 5.5. *We have the following convergence*

$$|X| + |X - P| - (|P| + b) \rightarrow |X| - \mathbf{m} \cdot X - b$$

with $\mathbf{m} = P/|P|$ as $|P| \rightarrow \infty$ uniformly for $X \in K \subset \mathbb{R}^3$ compact and $b \in I$ a bounded interval.

Proof. Set $\Delta = |X - P| + |P|$ and write

$$\begin{aligned} |X - P| - (|P| + b) &= \frac{|X - P|^2 - (|P| + b)^2}{\Delta + b} = \frac{|X|^2 - 2(X \cdot P + b|P|) - b^2}{\Delta + b} \\ &= \frac{|X|^2}{\Delta + b} - \frac{2|P|(X \cdot \mathbf{m} + b)}{\Delta + b} - \frac{b^2}{\Delta + b}. \end{aligned}$$

Since $\Delta = |X - |P|\mathbf{m}| + |P| = |P| \left(1 + \left|\frac{X}{|P|} - \mathbf{m}\right|\right)$, we have

$$\frac{\Delta + b}{2|P|} = \frac{1 + \left|\frac{X}{|P|} - \mathbf{m}\right|}{2} + \frac{b}{2|P|} \rightarrow 1$$

as $|P| \rightarrow \infty$, uniformly for X in a compact set and b in a bounded interval, the lemma follows. \blacksquare

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