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SCATTERING BY A BOUNDED HIGHLY OSCILLATING PERIODIC MEDIUM AND THE EFFECT OF BOUNDARY CORRECTORS*

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Abstract. We study the homogenization of a transmission problem arising in the scattering theory for bounded inhomogeneities with periodic coefficient in the lower-order term of the Helmholtz equation. The squared index of refraction is assumed to be a periodic function of the fast variable, specified over the unit cell with characteristic size ϵ. We obtain improved convergence results that assume lower regularity than previous estimates (which also allow for periodicity in the second-order operator), and we describe the asymptotic behavior of boundary correctors for general domains at all orders. In particular we show that, in contrast to Dirichlet problems, the $O(\epsilon)$ boundary corrector is nontrivial and can be observed in the far field. We further demonstrate the latter far field effect is larger than that of the "bulk" corrector—the so-called periodic drift, which is found to emerge only at $O(\epsilon^2)$. We illustrate the analysis by examples in one and two spatial dimensions.

Key words. periodic inhomogeneities, scattering, boundary layers, higher-order expansion

AMS subject classifications. 35R30, 35Q60, 35J40, 78A25

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1. Introduction.

Subwavelength manipulation of acoustic, electromagnetic, and elastic waves by periodic metamaterial structures caters for a broad range of applications including medical diagnosis [12], optical superfocusing [35], energy harvesting [36], and seismic protection [13]. In such endeavors the periodic structure is inherently (i) of finite extent and (ii) embedded in a reference "smooth" (say, homogeneous) medium, with its overall shape being driven by a diverse set of functionality requirements. While there is a large body of mathematics literature concerning the wave phenomena in unbounded periodic media [1, 2, 4, 8, 7, 14, 15, 20, 27, 32, 40], many unanswered questions remain about the role of the boundaries in scattering by compactly supported periodic structures. To help better understand the problem, we pursue the long-wavelength, low-frequency scattering by periodic (inhomogeneous) anomalies of compact support embedded in a homogeneous background. Recently, the classical theory of (two-scale) periodic homogenization for bounded domains has been adapted to deal with transmission problems in [11], including a study of the mean field equations and interfacial condition-driven boundary correctors. Unfortunately, explicit characterization of the boundary correctors in homogenization of periodic media has been notoriously difficult, in the case of both Dirichlet [3, 6, 16, 17, 22, 23, 24, 25, 26, 33, 34, 38] and transmission [11, 39] problems, as well

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as those featuring domains with small medium perturbations [29, 30, 31]. However, when the obstacle is periodic only in the refractive index, as is often the case in optical scattering, the most difficult aspect of the boundary corrector analysis disappears. For this class of configurations, we demonstrate that the boundary corrector effects can be both characterized explicitly and detected in the far field. We further show that, in contrast to Dirichlet problems, the boundary effect for transmission problems emerges already at $O(\epsilon)$, where ϵ is the vanishing size of the unit cell. These results, along with some simplifications and improvements upon the earlier convergence estimates, are the main contribution of this work.

The paper is organized as follows. In section 2 we introduce the problem, while in sections 3 and 4 we pursue the two-scale asymptotics as in [11] to establish the necessary mathematical framework and to expose the minimal regularity requirements. Section 3 focuses on the leading-order estimates, while section 4 highlights the analysis of higher-order terms. In section 5 we discuss the boundary correctors—including their limits on different domains, a general convergence theorem, and a remark concerning the germane inverse scattering problem. We illustrate the analysis by numerical examples in one and two spatial dimensions in sections 6 and 7, respectively.

2. Preliminaries. Let $D \subset \mathbb{R}^d$ for $d \geq 1$ be a bounded simply connected open set with piecewise-smooth boundary ∂D representing the support of a periodic inhomogeneity. In situations where ∂D is not smooth, we will in addition assume that D is convex [18, 19]. Next, let $\epsilon > 0$ be the characteristic size of the periodic unit cell, which is assumed to be small relative to both the size of D and the wavelength of the incident field, and let $Y = [0, 1]^d$ be the rescaled unit cell. We assume that the physical properties of an obstacle are given by a positive-definite *constant* a and a positive scalar *function* $n_\epsilon := n(x/\epsilon) \in L^\infty(D)$, related (in the context of acoustics) to the (isotropic) mass density and refraction index, respectively. Further, assume that n is periodic in $y = x/\epsilon$ with period Y. In what follows, $x \in D$ is referred to as the slow variable, while $y = x/\epsilon \in \mathbb{R}^d$ denotes the so-called fast variable [7]. We remark that our convergence analysis applies equally to a varying in the slow variable and to absorbing media, i.e., to complex a and n_ϵ; for simplicity, however, we focus our presentation on the case of real-valued coefficients. We additionally assume that $\inf_{|\xi|=1} \overline{\xi} \cdot a\xi = a_{min} > 0$ and $\inf_{y\in Y} n(y) > 0$. In this setting, the scattering of a time-harmonic incident field u^i by the above periodic inhomogeneity can be formulated for the total field, $u = u^s + u^i$, as

$$
\begin{aligned}
\nabla \cdot a\nabla u + k^2 n(x/\epsilon)u &= 0 \quad \text{in} \quad D,\\
\Delta u^s + k^2 u^s &= 0 \quad \text{in} \quad \mathbb{R}^d \setminus \overline{D},\\
\left(u^s + u^i\right) &= u \quad \text{on} \quad \partial D,\\
\nabla\left(u^s + u^i\right) \cdot \nu &= a\nabla u \cdot \nu \quad \text{on} \quad \partial D,
\end{aligned}
\tag{2.1}
$$

where u^s denotes the scattered field; the Sommerfeld radiation condition

$$
\lim_{r\to\infty} \sqrt{r}\left(\frac{\partial u^s}{\partial r} - iku^s\right) = 0
\tag{2.2}
$$

is satisfied uniformly with respect to $\hat{x} := x/|x|$, and ν is the outward unit normal on ∂D (see, e.g., [9]). In what follows we provide an asymptotic expansion for the above problem, including rigorous convergence estimates and the boundary corrector functions with their limits. The boundary corrector functions were quite difficult to analyze for periodic a, but in this case of a constant we will be able analyze their limits for general domains. Even in this case, however, the limit, if it exists, may still depend on how the sequence ϵ approaches zero, and the limiting boundary values will yield nontrivial effects in the far field in general.

3. Leading-order expansion of the transmission problem. The above scattering problem for an inhomogeneous obstacle D with periodically varying coefficients can be formulated as the transmission problem for $u_\epsilon := u$ in D and $u_\epsilon := u^s$ in $\mathbb{R}^d \setminus \overline{D}$, namely,

$$\begin{aligned} \nabla \cdot a\nabla u_\epsilon + k^2 n(x/\epsilon) u_\epsilon &= 0 \quad \text{in } D, \\ \Delta u_\epsilon + k^2 u_\epsilon &= 0 \quad \text{in } \mathbb{R}^d \setminus \overline{D}, \\ u_\epsilon^+ - u_\epsilon^- &= f \quad \text{on } \partial D, \\ (\nabla u_\epsilon \cdot \nu)^+ - (a\nabla u_\epsilon \cdot \nu)^- &= g \quad \text{on } \partial D, \end{aligned} \tag{3.1}$$

where u_ϵ satisfies the Sommerfeld radiation condition (2.2) at infinity. Here $f := -u^i$ and $g := -\nu \cdot \nabla u^i$ on ∂D, and the superscripts "+" and "−" denote the respective limits on ∂D from the exterior and interior of D. We are interested in developing the asymptotic theory for this problem as $\epsilon \to 0$, as was done for Dirichlet and Neumann problems on bounded domains [1, 7, 24, 33, 34]. As expected, we know [11] that the limiting problem is

$$\begin{aligned} \nabla \cdot a\nabla u_0 + k^2 \overline{n} u_0 &= 0 \quad \text{in } D, \\ \Delta u_0 + k^2 u_0 &= 0 \quad \text{in } \mathbb{R}^d \setminus \overline{D}, \\ u_0^+ - u_0^- &= f \quad \text{on } \partial D, \\ (\nabla u_0 \cdot \nu)^+ - (a\nabla u_0 \cdot \nu)^- &= g \quad \text{on } \partial D, \end{aligned} \tag{3.2}$$

where u_0 satisfies the Sommerfeld radiation condition (2.2) at infinity; $\overline{n}$ denotes the unit cell average of n, i.e.,

$$\overline{n} = \int_Y n(y)dy.$$

We will now rederive some of these results from [11], since we can obtain better estimates in this simpler case. While for the first-order corrections this analysis will seem like overkill, it will be convenient for the higher-order terms and boundary correctors. As before we use the standard technique which regards the solution as that depending on a "slow" variable x and a "fast" variable $y = x/\epsilon$ [7]. As was done in [33, 34], we write the equation for u_ϵ inside of D as a first-order system

$$\begin{aligned} a\nabla u_\epsilon - v_\epsilon &= 0, \\ \nabla \cdot v_\epsilon + k^2 n(x/\epsilon) u_\epsilon &= 0, \end{aligned} \tag{3.3}$$

which allows us to obtain (lower regularity) L^2-based estimates of the error. In this setting, an ansatz for the bulk expansions inside of D can be written as

$$\begin{aligned} u_\epsilon &= u_0(x, x/\epsilon) + \epsilon u^{(1)}(x, x/\epsilon) + \epsilon^2 u^{(2)}(x, x/\epsilon) + \dots, \\ v_\epsilon &= v_0(x, x/\epsilon) + \epsilon v^{(1)}(x, x/\epsilon) + \epsilon^2 v^{(2)}(x, x/\epsilon) + \dots. \end{aligned} \tag{3.4}$$

For the expansion in the exterior of D, there are no explicit microstructure terms. However, the exterior expansion will contain boundary corrector functions at all orders, and mean field terms beginning at second order, as in [11]. The boundary corrector functions solve problems which are substantially more difficult than our original; nonetheless they are necessary for full understanding of the behavior of the solution, even far from the boundary [7, 33]. However, in our case here of oscillating n only, their limits can be found explicitly, and we return to this issue later. We use the chain rule to write $\nabla = \nabla_x + \frac{1}{\epsilon}\nabla_y$, substitute (3.4) into (3.3), and equate the like powers of ϵ to obtain for the $O(1/\epsilon)$ terms

$$\nabla_y u_0 = 0 \tag{3.5}$$

and

$$\nabla_y \cdot v_0 = 0. \tag{3.6}$$

The $O(1)$ and $O(\epsilon)$ terms yield

$$v_0 - a\left(\nabla_y u^{(1)} + \nabla_x u_0\right) = 0, \tag{3.7}$$

$$\nabla_y \cdot v^{(1)} + \nabla_x \cdot v_0 + k^2 n(y) u_0 = 0, \tag{3.8}$$

$$v^{(1)} - a\left(\nabla_y u^{(2)} + \nabla_x u^{(1)}\right) = 0, \tag{3.9}$$

and

$$\nabla_y \cdot v^{(2)} + \nabla_x \cdot v^{(1)} + k^2 n(y) u^{(1)} = 0. \tag{3.10}$$

For our higher-order derivations we will also use

$$v^{(2)} - a\left(\nabla_y u^{(3)} + \nabla_x u^{(2)}\right) = 0, \tag{3.11}$$

$$\nabla_y \cdot v^{(3)} + \nabla_x \cdot v^{(2)} + k^2 n(y) u^{(2)} = 0, \tag{3.12}$$

$$v^{(3)} - a\left(\nabla_y u^{(4)} + \nabla_x u^{(3)}\right) = 0, \tag{3.13}$$

$$\nabla_y \cdot v^{(4)} + \nabla_x \cdot v^{(3)} + k^2 n(y) u^{(3)} = 0, \tag{3.14}$$

$$\vdots$$

from which one can see the general pattern. Equations (3.6) and (3.7) yield $u^{(1)} = u^{(1)}(x) = 0$ since the mean field (i.e., Y-cell average) of the first-order bulk correction has to vanish [11]. Note that here, unlike the case of periodically varying a, there are no first-order cell functions. The independence of $u^{(1)}$ on y and taking the Y-average of (3.8) yield the homogenized PDE in the interior of D (3.2). We also find the ith component of v_0 to read

$$(v_0(x))_i = \left(a\nabla_x u_0(x)\right)_i, \tag{3.15}$$

so the Y-average of v_0 is trivial, $\overline{v}_0 = \int_Y v_0 \,\mathrm{d}y = a\nabla u_0 = v_0$. From this, (3.15), (3.2), and (3.8), we get our first nontrivial bulk correction $\nabla_y \cdot v^{(1)} = k^2(\overline{n} - n(y))u_0$. We therefore define

$$v^{(1)} = k^2 a \nabla_y \beta(y) u_0, \tag{3.16}$$

where β is the unique zero-mean Y-periodic solution to

$$\nabla_y \cdot a\nabla_y \beta(y) \;=\; \overline{n} - n(y). \tag{3.17}$$

To summarize, we have formally derived that

$$u_\epsilon \approx u_0(x, x/\epsilon) + O\left(\epsilon^2\right),$$
$$v_\epsilon \approx v_0(x, x/\epsilon) + \epsilon v^{(1)}(x, x/\epsilon) + O\left(\epsilon^2\right),$$

where u_0, v_0, and $v^{(1)}$ in D are given respectively by (3.2), (3.15), and (3.16) in the interior of D. In the exterior of D, $v_0 = \nabla u_0$ and $v^{(1)}$ is zero. When we consider the proposed approximation for u_ϵ, we see that the Neumann type transmission conditions, which can be viewed as conditions on v_ϵ, are not quite exact due to the presence of $v^{(1)}$. It is for this reason that the above asymptotic expansions are not quite true in general without a boundary correction. This motivates the definition of our boundary corrector function θ_ϵ

$$\begin{aligned} \nabla \cdot a\nabla\theta_\epsilon + k^2 n(x/\epsilon)\theta_\epsilon &= 0 \quad \text{in } \; D,\\ \Delta\theta_\epsilon + k^2\theta_\epsilon &= 0 \quad \text{in } \; \mathbb{R}^d \setminus \overline{D},\\ \theta_\epsilon^+ - \theta_\epsilon^- &= 0 \quad \text{on } \; \partial D,\\ (\nabla\theta_\epsilon \cdot \nu)^+ - (a\nabla\theta_\epsilon \cdot \nu)^- &= v^{(1)} \cdot \nu \quad \text{on } \; \partial D, \end{aligned} \tag{3.18}$$

complemented by the Sommerfeld radiation condition (2.2) at infinity. From (3.16), the conormal transmission condition can be rewritten as

$$(\nabla\theta_\epsilon \cdot \nu)^+ - (a\nabla\theta_\epsilon \cdot \nu)^- = k^2 u_0 a \nabla_y \beta(x/\epsilon) \cdot \nu \quad \text{on } \; \partial D. \tag{3.19}$$

LEMMA 3.1. *Let u_ϵ be the solution to* (3.1) *and u_0 the solution to* (3.2), *and let the boundary correction θ_ϵ be given by* (3.18). *Then for any ball B_R of radius $R > 0$ which contains D,*

$$\|u_\epsilon - (u_0 + \epsilon\theta_\epsilon)\|_{H^1(B_R)} \le C_R \epsilon \|u_0\|_{H^1(D)},$$

where C_R is a constant independent of ϵ and u_0.

Proof. Introducing the auxiliary error functions in D as

$$z_\epsilon = u_\epsilon - u_0, \tag{3.20}$$

$$\eta_\epsilon = a\nabla u_\epsilon - v_0 - \epsilon v^{(1)}, \tag{3.21}$$

we find that from (3.15) we have $a\nabla z_\epsilon - \eta_\epsilon = \epsilon v^{(1)}$ and from (3.8) we obtain

$$-\nabla \cdot \eta_\epsilon = k^2 n(y)(u_\epsilon - u_0) + \epsilon k^2 \nabla_x \cdot (a\nabla_y \beta\, u_0) \tag{3.22}$$

$$= k^2 n(y) z_\epsilon + \epsilon k^2 a \nabla_y \beta \cdot \nabla u_0. \tag{3.23}$$

This shows that inside of D the error pair $(z_\epsilon, \eta_\epsilon)$ satisfies the first-order version of the PDEs with $O(\epsilon)$ residual. Outside of D we simply define $z_\epsilon = u_\epsilon - u_0$ and $\eta_\epsilon = \nabla z_\epsilon$, whereby $-\nabla \cdot \eta_\epsilon = k^2 z_\epsilon$. Now consider, for any $\phi \in C_0^\infty(B_R)$, the integral

$$\int_{B_R} (z_\epsilon - \epsilon\theta_\epsilon)\phi \, dx = \int_{B_R} (u_\epsilon - u_0 - \epsilon\theta_\epsilon)\, \phi \, dx, \tag{3.24}$$

and define the auxiliary function $W_\epsilon \in H^1_{loc}(\mathbb{R}^d)$ to solve

$$\begin{aligned} \nabla \cdot a\nabla W_\epsilon + k^2 n(x/\epsilon) W_\epsilon &= \phi \quad \text{in } \; D,\\ \Delta W_\epsilon + k^2 W_\epsilon &= \phi \quad \text{in } \; \mathbb{R}^d \setminus \overline{D},\\ W_\epsilon^+ - W_\epsilon^- &= 0 \quad \text{on } \; \partial D,\\ (\nabla W_\epsilon \cdot \nu)^+ - (a\nabla W_\epsilon \cdot \nu)^- &= 0 \quad \text{on } \; \partial D, \end{aligned} \tag{3.25}$$

together with the Sommerfeld radiation condition (2.2) at infinity. Note that this means that W_ϵ also satisfies the elliptic PDEs *across* ∂D with jumps in the coefficients. Then we have

$$\begin{aligned}\int_{B_R}(z_\epsilon-\epsilon\theta_\epsilon)\phi\,dx &= \int_D(z_\epsilon-\epsilon\theta_\epsilon)\left(\nabla\cdot a\nabla W_\epsilon+k^2n(x/\epsilon)W_\epsilon\right)\,dx\\ &\quad+\int_{B_R\setminus D}(z_\epsilon-\epsilon\theta_\epsilon)\left(\Delta W_\epsilon+k^2W_\epsilon\right)\,dx\\ &=-\int_D a\nabla z_\epsilon\cdot\nabla W_\epsilon\,dx+\epsilon\int_D a\nabla\theta_\epsilon\cdot\nabla W_\epsilon\,dx\\ &\quad+\int_D(z_\epsilon-\epsilon\theta_\epsilon)k^2n(x/\epsilon)W_\epsilon\,dx+\int_{\partial D}\nabla(z_\epsilon-\epsilon\theta_\epsilon)^+\cdot\nu W_\epsilon\,ds_x\\ &\quad+\int_{\partial B_R}(z_\epsilon-\epsilon\theta_\epsilon)\frac{\partial W_\epsilon}{\partial\nu}\,ds_x-\int_{\partial B_R}\frac{\partial(z_\epsilon-\epsilon\theta_\epsilon)}{\partial\nu}W_\epsilon\,ds_x,\end{aligned}$$

where we have integrated by parts once on the inside and twice on the exterior, using the fact that $(z_\epsilon-\epsilon\theta_\epsilon)$ exhibits no jump across ∂D. We also note that, by a standard argument, one can show that the last two terms on the outer boundary ∂B_R actually sum to zero since both $z_\epsilon-\epsilon\theta_\epsilon$ and W_ϵ satisfy the Sommerfeld radiation condition (2.2) at infinity. Indeed, all of the functions in the integrand satisfy the same Helmholtz equation in the exterior, so the last two terms can be integrated over a larger surface at some further radius R_1—on which the Sommerfeld condition can be used to show that the value of these integrals goes to zero as $R_1\to\infty$. Since no other terms depend on R_1, the original integrals must be zero [9]. Hence we have

$$\begin{aligned}\int_{B_R}(z_\epsilon-\epsilon\theta_\epsilon)\phi\,dx &= -\int_D a\nabla z_\epsilon\cdot\nabla W_\epsilon+\epsilon\int_D a\nabla\theta_\epsilon\cdot\nabla W_\epsilon\,dx\\ &\quad+\int_D(z_\epsilon-\epsilon\theta_\epsilon)k^2n(x/\epsilon)W_\epsilon\,dx+\int_{\partial D}\nabla(z_\epsilon-\epsilon\theta_\epsilon)^+\cdot\nu\,W_\epsilon\,ds_x.\end{aligned}$$

Now we use the differential equation (3.18) for θ_ϵ in the interior to obtain

$$\begin{aligned}\int_{B_R}(z_\epsilon-\epsilon\theta_\epsilon)\phi\,dx &= -\int_D a\nabla z_\epsilon\cdot\nabla W_\epsilon\,dx+\epsilon\int_{\partial D}(a\nabla\theta_\epsilon)^-\cdot\nu\,W_\epsilon\,dx\\ &\quad+\int_D z_\epsilon k^2n(x/\epsilon)W_\epsilon\,dx+\int_{\partial D}\nabla(z_\epsilon-\epsilon\theta_\epsilon)^+\cdot\nu\,W_\epsilon\,ds_x\end{aligned}$$

and use the normal jump for θ_ϵ from (3.18) to obtain

$$\begin{aligned}\int_{B_R}(z_\epsilon-\epsilon\theta_\epsilon)\phi\,dx &= -\int_D\eta_\epsilon\nabla W_\epsilon\,dx+\int_D z_\epsilon k^2n(x/\epsilon)W_\epsilon\,dx+\int_{\partial D}(\nabla z_\epsilon)^+\cdot\nu\,W_\epsilon\,ds_x\\ &\quad-\epsilon\int_D v^{(1)}\cdot\nabla W_\epsilon\,dx-\epsilon\int_{\partial D}v^{(1)}\cdot\nu\,W_\epsilon\,ds_x\\ &=-\epsilon k^2\int_D a\nabla_y\beta\cdot\nabla u_0W_\epsilon\,dx-\epsilon\int_D v^{(1)}\cdot\nabla W_\epsilon\,dx\\ &\quad-\int_{\partial D}\left(\epsilon(v^{(1)})^-\cdot\nu+(\eta_\epsilon)^-\cdot\nu-(\nabla z_\epsilon)^+\cdot\nu\right)W_\epsilon\,ds_x,\end{aligned}$$

where in the last step we integrated by parts and used (3.23). Now, using (3.21) and the normal jump conditions in (3.1) and (3.2), we see that the last boundary term above cancels (note that the boundary correction θ_ϵ was precisely chosen so that this would happen). Hence

$$\int_{B_R}(z_\epsilon - \epsilon\theta_\epsilon)\phi\,dx = -\epsilon k^2\int_D a\nabla_y\beta\cdot\nabla u_0\,W_\epsilon\,dx - \epsilon\int_D v^{(1)}\cdot\nabla W_\epsilon\,dx \tag{3.26}$$

for any $\phi \in C_0^\infty(B_R)$. Clearly from (3.16) and the boundedness of $\nabla_y\beta$ we have

$$\left\|v^{(1)}\right\|_{L^2(D)} \le C\|u_0\|_{L^2(D)} \tag{3.27}$$

for some C independent of ϵ. We also have

$$\|a\nabla_y\beta\cdot\nabla u_0\|_{L^2(D)} \le C\|u_0\|_{H^1(D)}.$$

Using the Cauchy–Schwarz inequality in (3.26) demonstrates that there exists constant C such that

$$\left|\int_{B_R}(z_\epsilon - \epsilon\theta_\epsilon)\phi\,dx\right| \le C\epsilon\|u_0\|_{H^1(D)}\|W_\epsilon\|_{H^1(D)}. \tag{3.28}$$

From standard elliptic estimates we have that

$$\|W_\epsilon\|_{H^1(D)} \le C_R\|\phi\|_{H^{-1}(B_R)},$$

where C_R depends only on the bounds on the coefficients, from which we obtain the desired result by inserting this into (3.28) and taking the supremum over all $\phi \in H^{-1}(B_R)$. ∎

The H^1 a priori estimate for the solution of the transmission problem (3.18) (see, e.g., Theorem 5.24 of [9]) implies that

$$\|\theta_\epsilon\|_{H^1(D)} + \|\theta_\epsilon\|_{H^1(B_R\setminus\overline{D})} \le C_R\left\|v^{(1)}\cdot\nu\right\|_{H^{-1/2}(\partial D)}. \tag{3.29}$$

Again since $\nabla\beta$ is bounded Y, one obtains

$$\left\|v^{(1)}\cdot\nu\right\|_{L^2(\partial D)} \le C\|u_0\|_{H^1(D)}. \tag{3.30}$$

Hence we find that

$$\|\theta_\epsilon\|_{H^1(D)} + \|\theta_\epsilon\|_{H^1(B_R\setminus D)} \le C_R\|u_0\|_{H^1(D)} \tag{3.31}$$

for some constant C_R independent of ϵ. Of course we also have

$$\|\theta_\epsilon\|_{L^2(B_R)} \le C_R\|u_0\|_{H^1(D)}. \tag{3.32}$$

From the above bounds we can obtain the following justification of the asymptotic expansion, where we note that unlike the case of oscillating a, we have $O(\epsilon)$ convergence in H^1 without any corrections.

THEOREM 3.2. *Let u_ϵ be the solution to* (3.1) *and u_0 the solution to* (3.2). *Then for any ball B_R of radius $R > 0$ which contains D,*

$$\|u_\epsilon - u_0\|_{H^1(D)} + \|u_\epsilon - u_0\|_{H^1(B_R\setminus D)} \le C_R\epsilon\|u_0\|_{H^1(D)}$$

and

$$\|u_\epsilon - u_0\|_{L^2(B_R)} \le C_R\epsilon\|u_0\|_{H^1(D)},$$

where C_R is a constant independent of ϵ.

4. Higher-order terms. In this section we pursue the asymptotic expansion further. We find the next terms in the bulk expansion and show implicitly that the first-order mean field correction discussed in [3, 7] vanishes in general. This was previously shown for problems with no lower-order terms [38, 33] and more generally in [11]. Here, both for completeness and to reduce the regularity requirements, we present a simplified proof for constant a and periodically varying n. If we apply a divergence operator $\nabla_y \cdot$ to (3.9), we obtain

$$\nabla_y \cdot a\nabla_y u^{(2)} \ = \ k^2(\overline{n} - n(y))u_0, \tag{4.1}$$

thanks to (3.8) and the homogenized equation for u_0. On recalling the fact that β is a unique zero-mean solution to (3.17), one verifies that

$$u^{(2)}(x,y) = k^2\beta(y)u_0 + \hat{u}^{(2)}(x) \tag{4.2}$$

indeed satisfies (4.1). Note that we have not yet determined the mean field $\hat{u}^{(2)}(x)$. From (3.9) we have, as before,

$$v^{(1)} = a\nabla_y u^{(2)} \ = \ k^2 a\nabla_y \beta(y)u_0. \tag{4.3}$$

We next find $u^{(3)}$ by taking the y divergence $\nabla_y \cdot$ of (3.11) and substituting back into (3.10) to obtain

$$\begin{aligned} \nabla_y \cdot a\nabla_y u^{(3)} &= -\nabla_x \cdot v^{(1)} - \nabla_y \cdot a\nabla_x u^{(2)} \\ &= -k^2 a\nabla_y \beta(y) \cdot \nabla u_0 - k^2 a\nabla_y \beta(y) \cdot \nabla u_0 \\ &= -2k^2 a\nabla_y \beta(y) \cdot \nabla u_0. \end{aligned} \tag{4.4}$$

We therefore define the new cell function γ to be the Y-periodic solution to

$$\nabla_y \cdot a\nabla_y \gamma = \beta \tag{4.5}$$

chosen to be the unique solutions with zero cell average $\int_Y \gamma dy = 0$. From this we obtain

$$u^{(3)} = -2k^2 a\nabla_y \gamma \cdot \nabla u_0 + \hat{u}^{(3)}(x) \tag{4.6}$$

and also from (3.11)

$$v^{(2)} = k^2\beta(y)a\nabla u_0 + a\nabla_x \hat{u}^{(2)} - 2k^2 a\left(\nabla_y^2\gamma\right)a\nabla u_0, \tag{4.7}$$

where the $\nabla_y^2\gamma$ represents the second-order derivative matrix of γ. Taking the x divergence of both sides in (4.7), plugging this into (3.12), and taking the Y cell average yields the equation for the mean field $\hat{u}^{(2)}$ inside D:

$$\left(\nabla \cdot a\nabla + k^2\overline{n}\right)\hat{u}^{(2)} = -k^4\overline{n\beta}u_0. \tag{4.8}$$

Unlike the oscillatory bulk corrections which are zero outside of D, we define $\hat{u}^{(2)}$ to be the unique solution to

$$\begin{aligned} \nabla \cdot a\nabla \hat{u}^{(2)} + k^2\overline{n}\hat{u}^{(2)} &= -k^4\overline{n\beta}u_0 \quad \text{in} \ \ D, \\ \Delta \hat{u}^{(2)} + k^2\hat{u}^{(2)} &= 0 \quad \text{in} \ \ \mathbb{R}^d \setminus \overline{D}, \\ \left(\hat{u}^{(2)}\right)^+ - \left(\hat{u}^{(2)}\right)^- &= 0 \quad \text{on} \ \ \partial D, \\ \left(\nabla \hat{u}^{(2)} \cdot \nu\right)^+ - \left(a\nabla \hat{u}^{(2)} \cdot \nu\right)^- &= 0 \quad \text{on} \ \ \partial D \end{aligned} \tag{4.9}$$

with the Sommerfeld radiation condition at infinity. Continuing with the ansatz, we take the y divergence of (3.13) and substitute in (3.12) to obtain the equation for $u^{(4)}$,

$$\begin{aligned}\nabla_y \cdot a\nabla_y u^{(4)} = k^2 \left(\overline{n} - n(y)\right) \hat{u}^{(2)} + k^4 \left(\overline{n}\beta(y) - n(y)\beta(y) + \overline{n\beta}\right) u_0 \\ + 4k^2 \left(a\nabla_y^2\gamma\right) : \left(a\nabla^2 u_0\right),\end{aligned} \tag{4.10}$$

where " : " denotes the matrix Frobenius product. Define new cell functions $\delta(y)$ and $\mu^{ik}(y)$ the Y-periodic, zero cell average solutions to

$$\nabla_y \cdot a\nabla_y \delta(y) = \overline{n\beta} - n(y)\beta(y) \tag{4.11}$$

and

$$\nabla_y \cdot a\nabla_y \mu^{ik}(y) = \frac{\partial^2\gamma}{\partial y_i \partial y_k} \tag{4.12}$$

so that

$$u^{(4)} = k^2\beta(y)\hat{u}^{(2)} + k^4(\overline{n}\gamma(y) + \delta(y))u_0 + 4k^2(a\mu) : \left(a\nabla^2 u_0\right) + \hat{u}^{(4)}(x). \tag{4.13}$$

From this and (3.13) we can directly obtain $v^{(3)}$. To find $\hat{u}^{(3)}$ we take the x divergence and Y cell average of (3.13) and substitute into the cell average of (3.14). We again choose $\hat{u}^{(3)}$ to have zero transmission data and be the unique solution to

$$\begin{aligned}\nabla \cdot a\nabla\hat{u}^{(3)} + k^2\overline{n}\hat{u}^{(3)} &= 2k^4\overline{na\nabla_y\gamma} \cdot \nabla u_0 \quad \text{in } D,\\ \Delta\hat{u}^{(3)} + k^2\hat{u}^{(3)} &= 0 \quad \text{in } \mathbb{R}^d \setminus \overline{D},\\ \left(\hat{u}^{(3)}\right)^+ - \left(\hat{u}^{(3)}\right)^- &= 0 \quad \text{on } \partial D,\\ \left(\nabla\hat{u}^{(3)} \cdot \nu\right)^+ - \left(a\nabla\hat{u}^{(3)} \cdot \nu\right)^- &= 0 \quad \text{on } \partial D.\end{aligned} \tag{4.14}$$

Since the mean field has no jumps across ∂D, it will not come into the boundary corrector. We are now ready to define the second-order boundary corrector, which we denote by $\theta_\epsilon^{(2)}$. Note that since $\overline{v}^{(1)}$, the Y cell average of $v^{(1)}$, and $u^{(1)}$, are both equal to zero, we can rewrite the equation for the first-order boundary corrector (3.18) as

$$\begin{aligned}\nabla \cdot a\nabla\theta_\epsilon + k^2 n(x/\epsilon)\theta_\epsilon &= 0 \quad \text{in } D,\\ \Delta\theta_\epsilon + k^2\theta_\epsilon &= 0 \quad \text{in } \mathbb{R}^d \setminus \overline{D},\\ \theta_\epsilon^+ - \theta_\epsilon^- = u^{(1)} - \hat{u}^{(1)} &= 0 \quad \text{on } \partial D,\\ (\nabla\theta_\epsilon \cdot \nu)^+ - (a\nabla\theta_\epsilon \cdot \nu)^- &= \left(v^{(1)} - \overline{v}^{(1)}\right) \cdot \nu \quad \text{on } \partial D.\end{aligned} \tag{4.15}$$

Similarly we define its second-order counterpart to solve

$$\begin{aligned}\nabla \cdot a\nabla\theta_\epsilon^{(2)} + k^2 n(x/\epsilon)\theta_\epsilon^{(2)} &= 0 \quad \text{in } D,\\ \Delta\theta_\epsilon^{(2)} + k^2\theta_\epsilon^{(2)} &= 0 \quad \text{in } \mathbb{R}^d \setminus \overline{D},\\ \theta_\epsilon^{(2)+} - \theta_\epsilon^{(2)-} &= u^{(2)} - \hat{u}^{(2)} \quad \text{on } \partial D,\\ \left(\nabla\theta_\epsilon^{(2)} \cdot \nu\right)^+ - \left(a\nabla\theta_\epsilon^{(2)} \cdot \nu\right)^- &= \left(v^{(2)} - \overline{v}^{(2)}\right) \cdot \nu \quad \text{on } \partial D,\end{aligned} \tag{4.16}$$

where here the Y cell average $\overline{v}^{(2)}$ is equal to $(a\nabla_x\hat{u}^{(2)})^- = (\nabla_x\hat{u}^{(2)})^+$ and is not zero in this case. We continue with the third order,

$$\begin{aligned}
\nabla \cdot a\nabla\theta_\epsilon^{(3)} + k^2 n(x/\epsilon)\theta_\epsilon^{(3)} &= 0 \quad \text{in} \quad D,\\
\Delta\theta_\epsilon^{(3)} + k^2\theta_\epsilon^{(3)} &= 0 \quad \text{in} \quad \mathbb{R}^d \setminus \overline{D},\\
{\theta_\epsilon^{(3)}}^+ - {\theta_\epsilon^{(3)}}^- &= u^{(3)} - \hat{u}^{(3)} \quad \text{on} \quad \partial D,\\
\left(\nabla\theta_\epsilon^{(3)} \cdot \nu\right)^+ - \left(a\nabla\theta_\epsilon^{(3)} \cdot \nu\right)^- &= \left(v^{(3)} - \overline{v}^{(3)}\right) \cdot \nu \quad \text{on} \quad \partial D.
\end{aligned} \tag{4.17}$$

At all orders, the boundary correctors $\theta_\epsilon^{(i)}$ will continue in the same pattern. For convenience, let us summarize the bulk terms we use in our expansion (all in the interior of D):

$$u^{(1)} = 0, \tag{4.18}$$

$$u^{(2)} = k^2\beta(y)u_0 \ + \ \hat{u}^{(2)}(x), \tag{4.19}$$

$$u^{(3)} = -2k^2 a\nabla_y\gamma \cdot \nabla_x u_0 + \hat{u}^{(3)}(x), \tag{4.20}$$

$$u^{(4)} = k^2\beta(y)\hat{u}^{(2)} + k^4\left(\overline{n}\gamma(y) + \delta(y)\right)u_0 + 4k^2(a\mu) : \left(a\nabla^2 u_0\right) + \hat{u}^{(4)}(x), \tag{4.21}$$

$$v_0 \ = a\nabla u_0(x), \tag{4.22}$$

$$v^{(1)} = ak^2\nabla_y\beta(y)u_0, \tag{4.23}$$

$$v^{(2)} = k^2\beta(y)a\nabla u_0 + a\nabla\hat{u}^{(2)} - 2k^2 a\left(\nabla_y^2\gamma\right)a\nabla u_0 \tag{4.24}$$

and

$$\begin{aligned}
v^{(3)} = {} & k^2 a\nabla_y\beta\hat{u}^{(2)} + k^4 a\nabla_y(\overline{n}\gamma + \delta)u_0\\
& + 4k^2 a\nabla_y\left((a\mu) : \left(a\nabla^2 u_0\right)\right) - 2k^2 a\left(\nabla^2 u_0\right)a\nabla_y\gamma + a\nabla_x\hat{u}^{(3)}.
\end{aligned} \tag{4.25}$$

In the exterior of D, all oscillating Y mean zero bulk terms are zero, while the homogenized solution u_0, $v_0 = \nabla u_0$ and the mean field terms $\hat{u}^{(i)}(x)$, and the boundary correctors $\theta_\epsilon^{(i)}$ extend to the far field based on their PDE definitions. The following theorem gives us a true second-order estimate of a solution to the transmission problem (3.1), assuming we have a bit more regularity on the homogenized solution.

LEMMA 4.1. *Let u_ϵ be the solution to* (3.1) *and u_0 the solution to* (3.2)*, and let the bulk and boundary corrections $u^{(2)}$,$u^{(3)}$, θ_ϵ, $\theta_\epsilon^{(2)}$, and $\theta_\epsilon^{(3)}$ be given respectively by* (4.19), (4.20), (4.15), (4.16)*, and* (4.17)*. Then for any ball B_R of radius $R > 0$ which contains D,*

$$\left\| u_\epsilon - \left(u_0 + \epsilon\theta_\epsilon + \epsilon^2 u^{(2)} + \epsilon^2\theta_\epsilon^{(2)}\right)\right\|_{H^1(B_R)} \le C_R\epsilon^2\|u_0\|_{H^2(D)}$$

and

$$\left\| u_\epsilon - \left(u_0 + \epsilon\theta_\epsilon + \epsilon^2 u^{(2)} + \epsilon^2\theta_\epsilon^{(2)} + \epsilon^3 u^{(3)} + \epsilon^3\theta_\epsilon^{(3)}\right)\right\|_{H^1(B_R)} \le C_R\epsilon^3\|u_0\|_{H^3(D)},$$

where C_R is a constant independent of ϵ and u_0.

Proof. We show the second result, as the proof is very similar to the proof of Lemma 3.1. We again define the error functions in D, but this time including the second- and third-order bulk corrections

$$z_\epsilon = u_\epsilon - u_0 - \epsilon^2 u^{(2)} - \epsilon^3 u^{(3)}, \tag{4.26}$$

$$\eta_\epsilon = a\nabla u_\epsilon - v_0 - \epsilon v^{(1)} - \epsilon^2 v^{(2)} - \epsilon^3 v^{(3)}. \tag{4.27}$$

In this case, one finds that

$$a\nabla z_\epsilon - \eta_\epsilon = \epsilon^3 \left(v^{(3)} - a\nabla_x u^{(3)}\right) \tag{4.28}$$

and

$$-\nabla\cdot\eta_\epsilon = k^2 n(x/\epsilon)\left(u_\epsilon - u_0 - \epsilon^2 u^{(2)}\right) + \epsilon^3\nabla_x\cdot v^{(3)} \tag{4.29}$$

$$= k^2 n(x/\epsilon) z_\epsilon + \epsilon^3\left(k^2 n(x/\epsilon)u^{(3)} + \nabla_x\cdot v^{(3)}\right). \tag{4.30}$$

Outside of D we have that $z_\epsilon = u_\epsilon - u_0 - \epsilon^2\hat{u}^{(2)} - \epsilon^3\hat{u}^{(3)}$ and $\eta_\epsilon = \nabla z_\epsilon$, and so $-\nabla\cdot\eta_\epsilon = k^2 z_\epsilon$. This shows that the error pair $(z_\epsilon, \eta_\epsilon)$ satisfies the first-order version of the PDE with an $O(\epsilon^3)$ residual inside, and exactly outside D (but not across the boundary). Consider, for any $\phi \in C_0^\infty(B_R)$, the integral

$$\begin{aligned}\int_{B_R}\left(z_\epsilon - \epsilon\theta_\epsilon - \epsilon^2\theta_\epsilon^{(2)} - \epsilon^3\theta^{(3)}\right)\phi\,dx &= \int_D\left(z_\epsilon - \epsilon\theta_\epsilon - \epsilon^2\theta_\epsilon^{(2)} - \epsilon^3\theta^{(3)}\right)\phi\,dx\\ &\quad+\int_{B_R\setminus D}\left(z_\epsilon - \epsilon\theta_\epsilon - \epsilon^2\theta_\epsilon^{(2)} - \epsilon^3\theta^{(3)}\right)\phi\,dx,\end{aligned} \tag{4.31}$$

and define the auxiliary function $W_\epsilon \in H^1_{loc}(\mathbb{R}^d)$ to solve (3.25) as before. Then, using the Sommerfeld radiation conditions to eliminate the outer boundary and the fact that $z_\epsilon - \epsilon\theta_\epsilon - \epsilon^2\theta_\epsilon^{(2)} - \epsilon^3\theta_\epsilon^{(3)}$ has no jump on ∂D, we find that

$$\begin{aligned}\int_{B_R}\left(z_\epsilon - \epsilon\theta_\epsilon - \epsilon^2\theta_\epsilon^{(2)} - \epsilon^3\theta_\epsilon^{(3)}\right)\phi\,dx &= -\int_D a\nabla z_\epsilon\cdot\nabla W_\epsilon\,dx\\ &\quad+\int_D a\nabla\left(\epsilon\theta_\epsilon + \epsilon^2\theta^{(2)} + \epsilon^3\theta^{(3)}\right)\cdot\nabla W_\epsilon\,dx\\ &\quad+\int_D\left(z_\epsilon - \epsilon\theta_\epsilon - \epsilon^2\theta_\epsilon^{(2)} - \epsilon^3\theta_\epsilon^{(3)}\right)n(x/\epsilon)W_\epsilon\,dx\\ &\quad+\int_{\partial D}\nabla\left(z_\epsilon - \epsilon\theta_\epsilon - \epsilon^2\theta_\epsilon^{(2)} - \epsilon^3\theta^{(3)}\right)^+\cdot\nu\,W_\epsilon\,ds_x.\end{aligned}$$

We now apply the differential equations for θ_ϵ, $\theta_\epsilon^{(2)}$, and $\theta_\epsilon^{(3)}$, their jump conditions, (4.28), and (4.29), which yield

$$\begin{aligned}\int_{B_R}&\left(z_\epsilon - \epsilon\theta_\epsilon - \epsilon^2\theta_\epsilon^{(2)} - \theta_\epsilon^{(3)}\right)\phi\,dx = -\int_D \eta_\epsilon\cdot\nabla W_\epsilon\,dx + \int_D z_\epsilon k^2 n(x/\epsilon)W_\epsilon\,dx\\ &+\int_{\partial D}(\nabla z_\epsilon)^+\cdot\nu\,W_\epsilon\,ds_x + \epsilon^3\int_D\left(-v^{(3)} + a\nabla_x u^{(3)}\right)\nabla W_\epsilon\,dx\\ &-\int_{\partial D}\left(\nabla\left(\epsilon\theta_\epsilon - \epsilon^2\theta_\epsilon^{(2)} - \epsilon^3\theta_\epsilon^{(3)}\right)^+\cdot\nu - a\nabla\left(\epsilon\theta_\epsilon + \epsilon^2\theta_\epsilon^{(2)} + \epsilon^3\theta_\epsilon^{(3)}\right)^-\cdot\nu\right)W_\epsilon\,ds_x\\ &= -\epsilon^3\int_D\left(k^2 n(x/\epsilon)u^{(3)} + \nabla_x\cdot v^{(3)}\right)W_\epsilon\,dx + \epsilon^3\int_D\left(-v^{(3)} + a\nabla_x u^{(3)}\right)\nabla W_\epsilon\,dx\\ &-\int_{\partial D}\left(\nabla\left(\epsilon\theta_\epsilon - \epsilon^2\theta_\epsilon^{(2)} - \epsilon^3\theta_\epsilon^{(3)}\right)^+\cdot\nu - a\nabla\left(\epsilon\theta_\epsilon + \epsilon^2\theta_\epsilon^{(2)} + \epsilon^3\theta_\epsilon^{(3)}\right)^-\cdot\nu\right)W_\epsilon ds_x\\ &+\int_{\partial D}\left((\eta_\epsilon\cdot\nu)^- - (\nabla z_\epsilon\cdot\nu)^+\right)W_\epsilon\,ds_x\\ &= -\epsilon^3\int_D\left(k^2 n(x/\epsilon)u^{(3)} + \nabla_x\cdot v^{(3)}\right)W_\epsilon\,dx + \epsilon^3\int_D\left(-v^{(3)} + a\nabla_x u^{(3)}\right)\nabla W_\epsilon dx,\end{aligned}$$

where in the last step the boundary integrals vanish thanks to the definitions of the three boundary correctors and (3.1), (3.2), (4.26), and (4.27). Note that here we are using more stringent regularity requirements on u_0 in order to secure boundedness of the above integrals. Indeed, the L^2 bounds on the featured integrands (in particular that on $\nabla_x \cdot v^{(3)}$) will require third-order L^2 derivatives, and we obtain

$$\left| \int_{B_R} \left(z_\epsilon - \epsilon\theta_\epsilon - \epsilon^2\theta_\epsilon^{(2)} - \epsilon^3\theta_\epsilon^{(3)} \right) \phi \, dx \right| \leq C\epsilon^3 \|u_0\|_{H^3(D)} \|W_\epsilon\|_{H^1(D)}. \tag{4.32}$$

Finally, the claim of the lemma follows from the bound

$$\|W_\epsilon\|_{H^1(D)} \leq C_R \|\phi\|_{H^{-1}(D)}$$

by taking the supremum over all $\phi \in H^{-1}(D)$. The first claim in the lemma follows from the exact proof as above, but without using the third-order terms in the definitions of z_ϵ and η_ϵ. The residuals in this case are $O(\epsilon^2)$ and depend only on second-order derivatives of u_0. ∎

Note that unlike the first-order boundary correctors, the higher-order ones have oscillating Dirichlet jumps which prevent them from being bounded in H^1. Following the same reasoning as that used to obtain the bound on θ_ϵ in [11], we have

$$\left\| \theta_\epsilon^{(2)} \right\|_{H^1(D)} + \left\| \theta_\epsilon^{(2)} \right\|_{H^1(B_R \setminus D)} \leq C_R \epsilon^{-1/2} \|u_0\|_{H^2(D)}, \tag{4.33}$$

$$\left\| \theta_\epsilon^{(3)} \right\|_{H^1(D)} + \left\| \theta_\epsilon^{(3)} \right\|_{H^1(B_R \setminus D)} \leq C_R \epsilon^{-1/2} \|u_0\|_{H^3(D)}, \tag{4.34}$$

$$\left\| \theta_\epsilon^{(2)} \right\|_{L^2(B_R)} \leq C_R \|u_0\|_{H^2(D)}, \tag{4.35}$$

and

$$\left\| \theta_\epsilon^{(3)} \right\|_{L^2(B_R)} \leq C_R \|u_0\|_{H^3(D)}. \tag{4.36}$$

Then the following theorem is a straightforward corollary of the above lemma.

THEOREM 4.2. *Let u_ϵ be the solution to* (3.1), *u_0 the solution to* (3.2), *and $u^{(2)}$ given by* (4.19) *and let the boundary corrections $\theta_\epsilon, \theta_\epsilon^{(2)}$ be given by* (4.15) *and* (4.16). *Then for any ball B_R of radius $R > 0$ which contains D, we have*

$$\|u_\epsilon - (u_0 + \epsilon\theta_\epsilon)\|_{L^2(B_R)} \leq C_R \epsilon^2 \|u_0\|_{H^2(D)}$$

and

$$\left\| u_\epsilon - \left(u_0 + \epsilon\theta_\epsilon + \epsilon^2 u^{(2)} + \epsilon^2 \theta_\epsilon^{(2)} \right) \right\|_{L^2(B_R)} \leq C_R \epsilon^3 \|u_0\|_{H^3(D)},$$

where C_R is a constant independent of ϵ and u_0.

5. Analysis of the boundary correctors. The boundary corrector (4.15) that comes in at first order for this problem is somewhat special due to the jump data being lower order; it is zero for the Dirichlet jump and bounded for the Neumann jump. In this case the added boundedness allows us to more easily obtain estimates with respect to ϵ. As one would expect, our candidate for the weak $L^2(B_R)$ limit of θ_ϵ is θ^*, which is the unique solution to

$$\begin{aligned} \nabla\cdot a\nabla\theta^* + k^2\overline{n}\theta^* &= 0 \quad \text{in} \quad D,\\ \Delta\theta^* + k^2\theta^* &= 0 \quad \text{in} \quad \mathbb{R}^d\setminus\overline{D},\\ {\theta^*}^+ - {\theta^*}^- &= 0 \quad \text{on} \quad \partial D,\\ (\nabla\theta^*\cdot\nu)^+ - (a\nabla\theta^*\cdot\nu)^- &= \overline{v^{(1)}}^{\partial}(x)\cdot\nu \quad \text{on} \quad \partial D, \end{aligned} \tag{5.1}$$

where

$$\overline{v^{(1)}}^{\partial}(x) := k^2 a(\nabla_y\beta)^* u_0(x), \tag{5.2}$$

where $(\nabla_y\beta)^*$ is the weak limit of $\nabla_y\beta(x/\epsilon)$ on ∂D as $\epsilon\to 0$.

LEMMA 5.1. *Let the first-order boundary corrector θ_ϵ be defined by* (4.15) *and θ^* by* (5.1), (5.2). *Then we have the convergence estimates*

$$\|\theta_\epsilon-\theta^*\|_{L^2(B_R)} \le C\left(\|\nabla_y\beta(x/\epsilon)\cdot\nu - (\nabla_y\beta)^*\cdot\nu\|_{H^{-1}(\partial D)} + \epsilon\right)\|u_0\|_{H^2(D)}$$

and

$$\begin{aligned} &\|\theta_\epsilon-\theta^*\|_{H^1(D)} + \|\theta_\epsilon-\theta^*\|_{H^1(B_R\setminus D)}\\ &\qquad \le C\left(\|\nabla_y\beta(x/\epsilon)\cdot\nu - (\nabla_y\beta)^*\cdot\nu\|_{H^{-1/2}(\partial D)} + \epsilon\right)\|u_0\|_{H^2(D)}. \end{aligned}$$

Proof. We introduce the intermediary function ψ_ϵ which satisfies

$$\begin{aligned} \nabla\cdot a\nabla\psi_\epsilon + k^2 n(x/\epsilon)\psi_\epsilon &= 0 \quad \text{in} \quad D,\\ \Delta\psi_\epsilon + k^2\psi_\epsilon &= 0 \quad \text{in} \quad \mathbb{R}^d\setminus\overline{D},\\ {\psi_\epsilon}^+ - {\psi_\epsilon}^- &= 0 \quad \text{on} \quad \partial D,\\ (\nabla\psi_\epsilon\cdot\nu)^+ - (a\nabla\psi_\epsilon\cdot\nu)^- &= \overline{v^{(1)}}^{\partial}(x)\cdot\nu \quad \text{on} \quad \partial D. \end{aligned}$$

Then, from Theorem 3.2 it follows that

$$\|\psi_\epsilon-\theta^*\|_{L^2(B_R)} \le C\epsilon\|u_0\|_{H^2(D)}$$

and

$$\|\psi_\epsilon-\theta^*\|_{H^1(D)} + \|\psi_\epsilon-\theta^*\|_{H^1(B_R\setminus D)} \le C\epsilon\|u_0\|_{H^2(D)}.$$

Now, from standard elliptic regularity for transmission problems, we have

$$\|\theta_\epsilon-\psi_\epsilon\|_{H^1(D)} + \|\theta_\epsilon-\psi_\epsilon\|_{H^1(B_R\setminus D)} \le C\|\nabla_y\beta(x/\epsilon)\cdot\nu-(\nabla_y\beta)^*\cdot\nu\|_{H^{-1/2}(\partial D)}\|u_0\|_{H^2(D)},$$

since both solve the same equation and differ only in the Neumann transmission data. Furthermore, from the proof of the L^2 estimates in the appendix in [11]

$$\|\theta_\epsilon-\psi_\epsilon\|_{L^2(B_R)} \le C\|\nabla_y\beta(x/\epsilon)\cdot\nu - (\nabla_y\beta)^*\cdot\nu\|_{H^{-1}(\partial D)}\|u_0\|_{H^2(D)},$$

and the result then follows from the triangle inequality. ∎

We now put together all of these results to obtain a theorem which gives the complete and computable first-order correction.

THEOREM 5.2. *Let u_ϵ be the solution to* (3.1) *and u_0 the solution to* (3.2), *and let the boundary correction θ^* be given by* (5.1). *Then for any ball B_R of radius $R>0$ which contains D, we have*

$$\begin{aligned} &\|u_\epsilon-(u_0+\epsilon\theta^*)\|_{H^1(D)} + \|u_\epsilon-(u_0+\epsilon\theta^*)\|_{H^1(B_R\setminus D)}\\ &\qquad \le C_R\epsilon\left(\|\nabla_y\beta(x/\epsilon)\cdot\nu - (\nabla_y\beta)^*\cdot\nu\|_{H^{-1/2}(\partial D)} + \epsilon^{1/2}\right)\|u_0\|_{H^2(D)} \end{aligned}$$

and

$$\|u_\epsilon - (u_0 + \epsilon\theta^*)\|_{L^2(B_R)} \le C_R\epsilon \left(\|\nabla_y\beta(x/\epsilon)\cdot\nu - (\nabla_y\beta)^*\cdot\nu\|_{H^{-1}(\partial D)} + \epsilon \right) \|u_0\|_{H^2(D)},$$

where C_R is a constant independent of ϵ and u_0.

5.1. Smooth domains. If D is a domain whose boundary has no flat parts of rational normal, then this limit $(\nabla_y\beta)^*$ will be its Y cell average, and therefore zero since it is the gradient of a Y-periodic function. In this case θ^* is identically zero. However, it is not in general true that $\|u_\epsilon - u_0\| = O(\epsilon^2)$, since the order of convergence of θ_ϵ to $\theta^* \equiv 0$ will depend on the particular geometry and may be slow. In order to correct for this effect, we introduce the intermediary boundary correction $\tilde{\theta}_\epsilon$ which satisfies

$$\begin{aligned} \nabla\cdot a\nabla\tilde{\theta}_\epsilon + k^2\overline{n}\tilde{\theta}_\epsilon &= 0 \quad \text{in} \;\; D, \\ \Delta\tilde{\theta}_\epsilon + k^2\tilde{\theta}_\epsilon &= 0 \quad \text{in} \;\; \mathbb{R}^d\setminus\overline{D}, \\ \tilde{\theta}_\epsilon^+ - \tilde{\theta}_\epsilon^- &= 0 \quad \text{on} \;\; \partial D, \\ \left(\nabla\tilde{\theta}_\epsilon\cdot\nu\right)^+ - \left(a\nabla\tilde{\theta}_\epsilon\cdot\nu\right)^- &= v^{(1)}\cdot\nu \quad \text{on} \;\; \partial D \end{aligned} \tag{5.3}$$

and note that $\tilde{\theta}_\epsilon$ has oscillatory boundary data, but a homogenized coefficient, so is much simpler to compute than θ_ϵ. From the proof of Theorem 3.2 it follows that

$$\left\|\theta_\epsilon - \tilde{\theta}_\epsilon\right\|_{H^1(D)} + \left\|\theta_\epsilon - \tilde{\theta}_\epsilon\right\|_{H^1(B_R\setminus D)} \le C_R\epsilon\left\|v^{(1)}\cdot\nu\right\|_{H^{-1/2}(\partial D)}$$

from which we can conclude from Theorem 4.2 that

$$\left\|u_\epsilon - (u_0 + \epsilon\tilde{\theta}_\epsilon)\right\|_{L^2(B_R)} \le C\epsilon^2\left\|u_0\right\|_{H^2(D)}.$$

In section 7 we demonstrate numerically for the case of a circular scatterer D that the boundary effects are larger than $O(\epsilon^2)$ and are corrected for with $\tilde{\theta}_\epsilon$.

5.2. Convex polygons. In the case where there is a flat part with rational normal, such as a convex polygon with sides of rational or infinite slope, the limit θ^* here will in general (i) depend on the sequence $\epsilon \to 0$ and (ii) not be zero, just as in [33]. This somehow degenerate case is quite common in applications, for example, when D is a union of period cells. In such a situation, the boundary data becomes one-dimensional periodic on each edge, and its boundary weak limit is the *boundary* cell average. That is, on each edge, the restriction of $\nabla_y\beta(x/\epsilon)\cdot\nu - (\nabla_y\beta)^*\cdot\nu$ is a periodic function with cell average zero, and so by the same arguments as in [33], [34], and [11],

$$\|\nabla_y\beta(x/\epsilon)\cdot\nu - (\nabla_y\beta)^*\cdot\nu\|_{H^{-1}(\partial D)} \le C\epsilon$$

and

$$\|\nabla_y\beta(x/\epsilon)\cdot\nu - (\nabla_y\beta)^*\cdot\nu\|_{H^{-1/2}(\partial D)} \le C\epsilon^{1/2}.$$

If additionally $a = 1$, the homogenized solution may still be smooth enough despite the corners, and one has the improved estimates

$$\begin{aligned} &\left\|u_\epsilon - \left(u_0 + \epsilon\theta^* + \epsilon^2 u^{(2)}\right)\right\|_{H^1(D)} + \left\|u_\epsilon - \left(u_0 + \epsilon\theta^* + \epsilon^2 u^{(2)}\right)\right\|_{H^1(B_R\setminus D)} \\ &\qquad \le C_R\epsilon^{3/2}\|u_0\|_{H^3(D)} \end{aligned}$$

and

$$\|u_\epsilon - (u_0 + \epsilon\theta^*)\|_{L^2(B_R)} \le C_R \epsilon^2 \|u_0\|_{H^2(D)}. \tag{5.4}$$

We note, however, that for general a one does not have such regularity. In such a case, for $u_0 \in H^{1+s}(D)$ and $0 < s < 1$ one could interpolate between Lemma 3.1 and (5.4) just as in [33] and obtain the error estimate

$$\|u_\epsilon - (u_0 + \epsilon\theta^*)\|_{L^2(B_R)} \le C_R \epsilon^{1+s} \|u_0\|_{H^{1+s}(D)}. \tag{5.5}$$

5.3. General boundary correctors. At each higher order ϵ^i, one will have a bulk correction $u^{(i)}, v^{(i)}$ which includes its mean field $\hat{u}^{(i)}, \overline{v}^{(i)}$. The mean field will be defined to have no transmission jumps, and ith-order boundary corrector will be the unique solution to

$$\begin{aligned} \nabla \cdot a \nabla \theta_\epsilon^{(i)} + k^2 n(x/\epsilon)\theta_\epsilon^{(i)} &= 0 \quad \text{in } \ D, \\ \Delta \theta_\epsilon^{(i)} + k^2 \theta_\epsilon^{(i)} &= 0 \quad \text{in } \ \mathbb{R}^d \setminus \overline{D}, \\ {\theta_\epsilon^{(i)}}^+ - {\theta_\epsilon^{(i)}}^- &= u^{(i)} - \hat{u}^{(i)} \quad \text{on } \ \partial D, \\ \left(\nabla \theta_\epsilon^{(i)} \cdot \nu\right)^+ - \left(a \nabla \theta_\epsilon^{(i)} \cdot \nu\right)^- &= \left(v^{(i)} - \overline{v}^{(i)}\right) \cdot \nu \quad \text{on } \ \partial D, \end{aligned} \tag{5.6}$$

where the transmission data consists only of the bulk corrections. For the higher-order corrections we do not obtain estimates as easily as for the first-order term. Due to the presence of the oscillatory Dirichlet jump, $\theta_\epsilon^{(i)}$ are $O(\epsilon^{-1/2})$ in H^1 for $i \ge 2$. However, they do converge in L^2 as we see in the following theorem.

THEOREM 5.3. *Let the ith-order boundary corrector be given by* (5.6)*, and assume that the boundary data are bounded uniformly in $L^2(\partial D)$. Assume $\epsilon_k \to 0$ is a sequence such that weak limits of $u^{(i)} - \hat{u}^{(i)}$ and $v^{(i)} - \overline{v}^{(i)}$ exist on $L^2(\partial D)$, call them $u^{(i)*}$ and $v^{(i)*}$. Then if ∂D is smooth or $a = 1$, $\theta_{\epsilon_k}^{(i)}$ converges strongly in $L^2(B_R)$ to $\theta^{(i)*}$, the unique solution to*

$$\begin{aligned} \nabla \cdot a \nabla \theta^{(i)*} + k^2 \overline{n} \theta^{(i)*} &= 0 \quad \textit{in } \ D, \\ \Delta \theta^{(i)*} + k^2 \theta^{(i)*} &= 0 \quad \textit{in } \ \mathbb{R}^d \setminus \overline{D}, \\ {\theta^{(i)*}}^+ - {\theta^{(i)*}}^- &= u^{(i)*} \quad \textit{on } \ \partial D, \\ \left(\nabla \theta^{(i)*} \cdot \nu\right)^+ - \left(a \nabla \theta^{(i)*} \cdot \nu\right)^- &= v^{(i)*} \cdot \nu \quad \textit{on } \ \partial D. \end{aligned} \tag{5.7}$$

Remark 5.1. Note that here we assume uniform L^2 boundedness of the boundary data. It is necessary to make this assumption because the expressions for $u^{(i)}$ and $v^{(i)}$ involve derivatives of u_0, which in the case when D is not C^∞ might not be bounded in $L^2(\partial D)$. There is no issue with the oscillations, so for C^∞ boundaries this assumption will always hold.

Proof. For simplicity we leave off the (i) superscripts. Given $\phi \in C_0^\infty(B_R)$, define $W_\epsilon \in H^1_{\text{loc}}(\mathbb{R}^d)$ to solve (3.25). Consider

$$\begin{aligned} \int_{B_R} \theta_\epsilon \phi \, dx &= \int_D \theta_\epsilon \left(\nabla \cdot a \nabla W_\epsilon + k^2 n W_\epsilon\right) dx + \int_{B_r \setminus D} \theta_\epsilon \left(\Delta W_\epsilon + k^2 W_\epsilon\right) dx \\ &= \int_{\partial D} (u - \hat{u})(a \nabla W_\epsilon \cdot \nu)^- ds_x + \int_{\partial D} (v - \overline{v}) \cdot \nu W_\epsilon ds_x \end{aligned}$$

by application integration by parts twice and the jump data for θ_ϵ. Similarly, the conjectured limit θ^* satisfies

$$\int_{B_R} \theta^* \phi \, dx = \int_{\partial D} u^* (a\nabla W_0 \cdot \nu)^- ds_x + \int_{\partial D} v^* \cdot \nu W_0 ds_x,$$

where W_0 solves the homogenized version of (3.25). Subtracting these and adding and subtracting appropriate terms, we obtain

$$\begin{aligned}\int_{B_R} (\theta_\epsilon - \theta^*)\phi \, dx = &\int_{\partial D} (u - \hat{u})(a\nabla W_\epsilon \cdot \nu - a\nabla W_0 \cdot \nu)^- \, ds_x \\ &+ \int_{\partial D} (u - \hat{u} - u^*)(a\nabla W_0)^- \, ds_x + \int_{\partial D} (v - \overline{v})(W_\epsilon - W_0) ds_x \\ &+ \int_{\partial D} (v - \overline{v} - v^*) W_0 ds_x.\end{aligned}$$

Note that $W_\epsilon \to W_0$, and from Theorem 3.2, this convergence is strong in $H^1(D)$. This means that $W_\epsilon \to W_0$ strongly in $L^2(\partial D)$ by the trace theorem. Furthermore, since either ∂D is smooth or $a = 1$, we have that W_ϵ is in $H^2(D)$ and is in fact bounded there uniformly by $\|W_\epsilon\|_{H^2(D)} \le C\|\phi\|_{L^2(D)}$. This then implies that $(a\nabla W_\epsilon \cdot \nu)^-$ is bounded in $H^{1/2}(\partial D)$ and therefore bounded (indeed precompact) in $L^2(\partial D)$. Now we can bound

$$\begin{aligned}\left|\int_{B_R} (\theta_\epsilon - \theta^*) \, \phi \, dx\right| \le\; &\|(u - \hat{u})\|_{L^2(\partial D)} \|(a\nabla W_\epsilon \cdot \nu)^- - (a\nabla W_0 \cdot \nu)^-\|_{L^2(\partial D)} \\ &+ \|(u - \hat{u} - u^*)\|_{H^{-1/2}(\partial D)} \|(a\nabla W_0 \cdot \nu)^-\|_{H^{1/2}(\partial D)} \\ &+ \|(v - \overline{v})\|_{L^2(\partial D)} \|W_\epsilon - W_0\|_{L^2(\partial D)} \\ &+ \|(v - \overline{v} - v^*)\|_{H^{-3/2}(\partial D)} \|W_0\|_{H^{3/2}(\partial D)}.\end{aligned} \tag{5.8}$$

From Theorem 3.2, we have that $\|W_\epsilon - W_0\|_{H^1(D)} \le C\epsilon\|\phi\|_{L^2(B_R)}$, along with $\|W_\epsilon - W_0\|_{H^2(D)} \le C\|\phi\|_{L^2(B_R)}$. From interpolation, this means that $\|W_\epsilon - W_0\|_{H^{3/2+\delta}(D)} \le C_\epsilon\|\phi\|_{L^2(B_R)}$, where $C_\epsilon \to 0$ as $\epsilon \to 0$. From the trace theorem the same bound holds on their normal derivatives on the boundary in H^δ and therefore also in L^2. Hence we have from the trace theorem and the above mentioned results that

$$\begin{aligned}\left|\int_{B_R} (\theta_\epsilon - \theta^*)\phi \, dx\right| \le\; &\|(u - \hat{u})\|_{L^2(\partial D)} C_\epsilon \|\phi\|_{L^2(B_R)} \\ &+ C\|(u - \hat{u} - u^*)\|_{H^{-1/2}(\partial D)} \|\phi\|_{L^2(B_R)} \\ &+ \|(v - \overline{v})\|_{L^2(\partial D)} C\epsilon \|\phi\|_{L^2(B_R)} \\ &+ C\|(v - \overline{v} - v^*)\|_{H^{-3/2}(\partial D)} \|\phi\|_{L^2(B_R)}.\end{aligned} \tag{5.9}$$

Dividing by $\|\phi\|_{L^2(B_R)}$ and taking the supremum, we have that

$$\begin{aligned}\|\theta_\epsilon - \theta^*\|_{L^2(B_R)} \le\; &C_\epsilon \|(u - \hat{u})\|_{L^2(\partial D)} + C\|(u - \hat{u} - u^*)\|_{H^{-1/2}(\partial D)} \\ &+ C\epsilon\|(v - \overline{v})\|_{L^2(\partial D)} + C\|(v - \overline{v} - v^*)\|_{H^{-3/2}(\partial D)},\end{aligned} \tag{5.10}$$

where $C_\epsilon \to 0$. Furthermore, since the boundary data is bounded in $L^2(\partial D)$ and converging weakly, from the compact embedding of $L^2(\partial D)$ into $H^{-1/2}(\partial D)$, all subsequences have a subsequence which converges strongly in $H^{-1/2}$, and so due to the uniqueness of the weak limit the entire sequence must converge strongly in $H^{-1/2}$ and of course also in $H^{-3/2}$. Hence all terms on the right-hand side of (5.10) converge to zero. ∎

We expect the above result also holds for D any convex polygon; however, some details need to be checked due to the lack of H^2 estimates if a is not the identity. If the sides of the D have normal rational to the periodic structure, the proof of Theorem 4.1 in [11] may be used, and of course in this case the limit is not in general unique.

5.4. A remark about inversion. A natural question to ask is if one can use the expansion $u_\epsilon(x) \approx u_0 + \epsilon\tilde{\theta}_\epsilon$ as a model for far field measurements to recover properties of $n(x)$. From standard integration by parts we can see that we can write $\tilde{\theta}_\epsilon$ as the single layer potential

$$\tilde{\theta}_\epsilon(z) = k^2 \int_{\partial D} a\nabla_y \beta(x/\epsilon) \cdot \nu u_0(x) G^{a,\overline{n}}(z,x) d\sigma_x,$$

where $G^{a,\overline{n}}$ is the fundamental solution corresponding to a background with the homogenized scatterer embedded. Assuming one knows $D, a, \overline{n}$, perhaps from qualitative reconstruction methods [10], this formula can potentially be used to recover $a\nabla_y\beta \cdot \nu$ on ∂D. However, further inspection reveals that since $\nabla_y \cdot a\nabla_y\beta = \overline{n} - n$,

$$\epsilon\tilde{\theta}_\epsilon(z) = k^2 \int_D (\overline{n} - n(x/\epsilon)) u_0(x) G^{a,\overline{n}}(z,x) dx + O\left(\epsilon^2\right),$$

revealing that $u_0 + \epsilon\tilde{\theta}_\epsilon$ is, up to $O(\epsilon^2)$ error, simply the Born approximation for u_ϵ viewed as a perturbation of the homogenized background solution. This coincides with what one would expect if we have the correct linearization. Below we demonstrate what one can recover in one dimension.

6. One-dimensional problem.

6.1. Solution expansion. We now compute solutions for a one-dimensional example in detail. Let $D = (0,1)$, $a = 1$ for simplicity, and compute the solution $u_\epsilon(x)$ to

$$\begin{aligned} u_\epsilon'' + k^2 n(x/\epsilon) u_\epsilon &= 0 \quad \text{if } x \in (0,1), \\ u_\epsilon'' + k^2 u_\epsilon &= 0 \quad \text{otherwise,} \end{aligned} \tag{6.1}$$

with the Sommerfeld radiation condition at infinity, and $u_{\mathbf{i}} = e^{ikx}$. In one dimension, the Sommerfeld condition implies that the scattered field solution outside of D takes the form

$$u_\epsilon(x) = c_1^\epsilon e^{-ikx} \quad \text{for } x < 0 \quad \text{and} \quad u_\epsilon(x) = c_2^\epsilon e^{ikx} \quad \text{for } x > 1.$$

Continuity of the total field across the boundary of D implies that c_1^ϵ and c_2^ϵ are given by

$$c_1^\epsilon = u_\epsilon^-(0) - 1 \quad \text{and} \quad c_2^\epsilon = u_\epsilon^-(1)e^{-ik} - 1,$$

where the $-$ refers to the value of u_ϵ from the interior of D, and continuity of the derivative of the total field allows us to convert the problem to one in the interior of D with Robin boundary conditions:

$$\begin{aligned} u_\epsilon'' + k^2 n(x/\epsilon) u_\epsilon = 0 \quad \text{for } x \in (0,1), \\ u_\epsilon'(0) + iku_\epsilon(0) = 2ik \quad u_\epsilon'(1) - iku_\epsilon(1) = 0, \end{aligned} \tag{6.2}$$

which we can solve numerically. The homogenized solution $u_0(x)$ likewise solves

$$\begin{aligned} u_0'' + k^2 \overline{n} u_0 = 0 \quad \text{for } x \in (0,1), \\ u_0'(0) + iku_0(0) = 2ik \quad u_0'(1) - iku_0(1) = 0, \end{aligned} \tag{6.3}$$

which we can solve explicitly. In D,

$$u_0(x) = \frac{2\left(\sqrt{\overline{n}}+1\right)e^{ik\sqrt{\overline{n}}(x-1)} + 2\left(\sqrt{\overline{n}}-1\right)e^{-ik\sqrt{\overline{n}}(x-1)}}{\left(\sqrt{\overline{n}}+1\right)^2 e^{-ik\sqrt{\overline{n}}} - \left(\sqrt{\overline{n}}-1\right)^2 e^{ik\sqrt{\overline{n}}}} \tag{6.4}$$

and of course outside $u_0 = c_1 e^{-ikx}$ for $x < 0$ and $u_0 = c_2 e^{ikx}$ for $x > 1$, where c_1 and c_2 are given by $c_1 = u_0(0) - 1$ and $c_2 = u_0(1)e^{-ik} - 1$. The boundary corrector $\theta_\epsilon(x)$ also satisfies a similar Robin problem, but with the prescribed Neumann jump given by $v^{(1)}$,

$$\theta_\epsilon'' + k^2 n(x/\epsilon)\theta_\epsilon = 0 \quad \text{in} \quad (0,1),$$
$$\theta_\epsilon'(0) + ik\theta_\epsilon(0) = -k^2 u_0(0)\beta'(0), \quad \theta_\epsilon'(1) - ik\theta_\epsilon(1) = -k^2 u_0(1)\beta'(1/\epsilon).$$

We compute in one dimension that $\beta(y)$ is given on $(0,1)$ by

$$\beta'(y) = \int_0^y (\overline{n} - n(s))\, ds - \int_0^1 \int_0^y (\overline{n} - n(s))\, dsdy$$

and is extended periodically. One can see from the boundary conditions that θ_ϵ does not have a unique limit for general sequences of $\epsilon \to 0$, as in [33]. However, for a given finite ϵ, there is a corresponding subsequential limit which has the same boundary cutoff. That is to say, any $\epsilon > 0$ can be written as $\frac{1}{N+\delta}$, where $N \in \mathbb{Z}$ and $\delta \in [0,1)$, and the subsequential limits are characterized by δ. We write the limiting boundary corrector (corresponding to cutoff δ) as $\theta^*(x)$, the solution to

$$(\theta^*)'' + k^2\overline{n}\theta^* = 0 \quad \text{in} \quad (0,1),$$
$$(\theta^*)'(0) + ik\theta^*(0) = -k^2 u_0(0)\beta'(0), \quad (\theta^*)'(1) - ik\theta^*(1) = -k^2 u_0(1)\beta'(\delta).$$

Which we can solve explicitly. Numerical results from Figure 6.1 show that θ^* is sufficient to act as the boundary corrector in the approximation for the true solution $u_\epsilon(x)$. Note that we obtain an order of convergence $O(\epsilon^2)$ with the addition of $\epsilon\theta_\epsilon$ or $\epsilon\theta^*$ and an order of convergence $O(\epsilon)$ without a boundary corrector. For the second-order expansion in the bulk, we have an oscillatory term and a drift term

$$u^{(2)}(x) = k^2\beta(x/\epsilon)u_0 + \hat{u}^{(2)}(x),$$

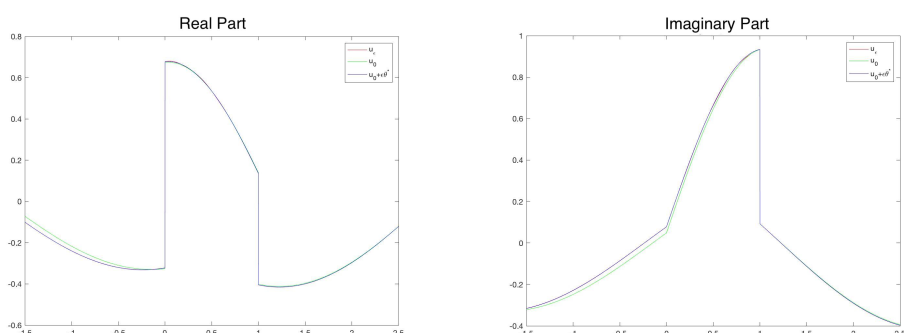

FIG. 6.1. *Real and imaginary parts of u_ϵ (red) versus first-order approximations u_0 (green) and $u_0 + \epsilon\theta^*$ (blue) assuming $n(y) = 2 + \sin(2\pi y)$, $\epsilon = 1/3.1$, and $k = 1$. Note that the red and blue lines are indistinguishable.*

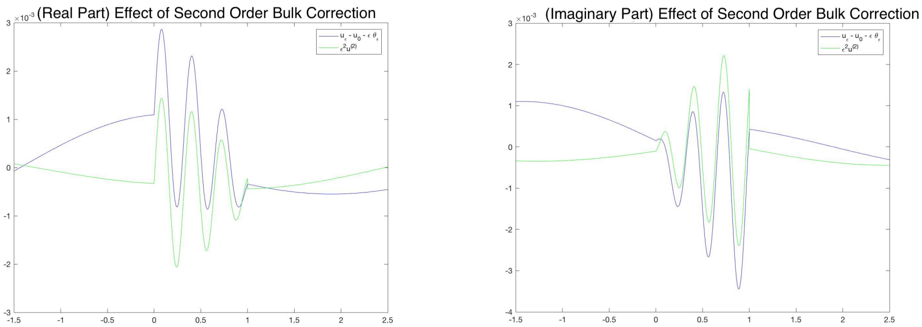

FIG. 6.2. *Real and imaginary parts of the first-order error* $u_\epsilon - (u_0 + \epsilon\theta_\epsilon)$ *(blue) versus second-order bulk correction* $\epsilon^2 u^{(2)}$ *(green) assuming* $n(y) = 2 + \sin(2\pi y)$*,* $\epsilon = 1/3.1$*, and* $k = 1$*.*

where $\hat{u}^{(2)}$ solves

$$\left(\hat{u}^{(2)}\right)'' + k^2 \overline{n} \hat{u}^{(2)} = -k^4 \overline{n\beta} u_0 \quad \text{on} \quad (0, 1),$$

with Helmholtz outside, no jumps across the boundary, and the Sommerfeld radiation condition at infinity. We include plots of the real and imaginary parts of $u^{(2)}$ alongside the real and imaginary parts of the error between u_ϵ and $u_0 + \epsilon\theta_\epsilon$ for $\epsilon = 1/3.1$ in Figure 6.2. Notice that $u^{(2)}$ is accurately correcting for the oscillations and the drift, but a boundary term is missing, and its effect propagates into the far field, as in the first-order term. Furthermore, these second-order boundary effects are on the same order as the drift $\hat{u}^{(2)}$.

The second-order boundary corrector $\theta_\epsilon^{(2)}$ also solves a Robin problem on D,

$$\begin{aligned}
&\left(\theta_\epsilon^{(2)}\right)'' + k^2 n(x/\epsilon) \theta_\epsilon^{(2)} = 0 \quad \text{on} \quad D, \\
&\left(\theta_\epsilon^{(2)}\right)'(0) + ik\theta_\epsilon^{(2)}(0) = k^2 \beta(0) u_0'(0) - ik^3 \beta(0) u_0(0), \\
&\left(\theta_\epsilon^{(2)}\right)'(1) - ik\theta_\epsilon^{(2)}(1) = k^2 \beta(1/\epsilon) u_0'(1) + ik^3 \beta(1/\epsilon) u_0(1).
\end{aligned}$$

For our particular $n(y)$, $\theta_\epsilon^{(2)}$ is zero for $\epsilon = 1/N$, $N \in \mathbb{Z}$, although this is not generally true for any choice of n. Indeed, we observe an order of convergence $O(\epsilon^3)$ when adding $\epsilon^2\theta_\epsilon^{(2)}$, and in general only $O(\epsilon^2)$ without it. In these computations θ_ϵ is used in the first-order correction, not θ^*; such a replacement would have resulted in another second-order term. This could be computed easily in one dimension, but we do not do that here.

6.2. Far field expansion and inversion. Let us assume now that one can read the solution u_ϵ of (6.1) in the far field. We saw earlier that we have an explicit first-order expansion for the solution in the far field

$$u_\epsilon(x) \approx u_0 + \epsilon\theta^*(x) = \begin{cases} c_1 e^{-ikx}, & x < 0, \\ c_2 e^{ikx}, & x > 1, \end{cases}$$

where c_1 and c_2 can be written in the form

$$c_1 = A_1\left(\overline{n}, e^{ik\sqrt{\overline{n}}}\right) + \epsilon k\beta'(0)B_1\left(\overline{n}, e^{ik\sqrt{\overline{n}}}\right) + \epsilon k\beta'(\delta)C_1\left(\overline{n}, e^{ik\sqrt{\overline{n}}}\right),$$
$$c_2 = A_2\left(\overline{n}, e^{ik\sqrt{\overline{n}}}\right) + \epsilon k\beta'(0)B_2\left(\overline{n}, e^{ik\sqrt{\overline{n}}}\right) + \epsilon k\beta'(\delta)C_2\left(\overline{n}, e^{ik\sqrt{\overline{n}}}\right),$$

where A_l, B_l, C_l, $l = 1, 2$, are functions only of $\overline{n}$ and $e^{ik\sqrt{\overline{n}}}$ which can be found analytically. Assuming one knows the location of the scatterer D and can control the incident wave (i.e., control k), one can use the above expansion to recover $\overline{n}$, $\epsilon\beta'(0)$, and $\epsilon\beta'(\delta)$. Note that $\beta'(0)$ and $\beta'(\delta)$ can be considered as measures of how far n deviates from its average. In the recovery below, we assume we know ϵ and recover the unknowns as expected, although we note that this is without adding any noise. Furthermore, by using the formulas for A_l, B_l, C_l, if one were to use the second-order ϵ^2 far field information, one could potentially additionally recover $\overline{n\beta}$, $\beta(0)$, and $\beta(\delta)$. For this, however, one would also need to find the first-order correction for θ_ϵ to obtain the entire $O(\epsilon^2)$ term.

Inversion assuming $n(y) = \overline{n} + \sin(2\pi y)$ and $\epsilon = 1/3$.

	$\overline{n}$	$\beta'(0)$	$\beta'(\delta)$
Actual	2	0.1591549	0.1591549
Recovered	1.999033	0.1696745	0.1564401
Error	9.6675e-4	0.0105196	0.0027149
Actual	4	0.1591549	0.1591549
Recovered	4.000289	0.1682484	0.1641211
Error	2.8856e-4	0.0090934	0.0049661

Inversion assuming $n(y) = \overline{n} + \sin(2\pi y)$ and $\epsilon = 1/10$.

	$\overline{n}$	$\beta'(0)$	$\beta'(\delta)$
Actual	2	0.1591549	0.1591549
Recovered	1.999204	0.1631196	0.1541649
Error	7.9578e-4	0.0039646	0.0049901
Actual	4	0.1591549	0.1591549
Recovered	4.000361	0.1589694	0.1600673
Error	3.6087e-4	1.8554e-4	9.1239e-4

7. Numerical examples in two dimensions.

7.1. Square domain. We first consider a smoothly varying periodic n on a square. Let $D = (-0.5, 0.5)^2$, $a = I$ (the identity), and consider the solution to (3.1) with

$$n(y) = 2 + \sin(2\pi y_1) + \cos(2\pi y_2).$$

Assume the incident wave u_i is given by e^{ikx}. We numerically compute the scattered solution u_s using cubic finite elements with perfectly matched layers to model the radiation boundary conditions. The scattered field of the homogenized solution solving (3.2) can be computed similarly.

Recall that, as in one dimension, the limit θ^* is not unique here due to the flat boundary cutting the period cell at a rational normal. Assume we have a subsequential limit of θ_ϵ, that is, we consider a sequence $\{\epsilon_\delta\}$ where $\epsilon_\delta = \frac{1}{N+\delta}$ for a fixed $\delta \in [0, 1)$ with $N \in \mathbb{Z}$. Recall that θ^* is the unique solution to (5.1), with boundary data corresponding to cutoff δ. We solve for β, the solution to (3.17), numerically using quadratic finite elements.

Numerical results in Figures 7.1–7.3 show that θ^* is sufficient to act as the boundary corrector in the approximation for the true solution u_ϵ. In all figures we are plotting the scattered field both inside and outside of the scatterer. In Figure 7.4, we plot $\log_2(\epsilon)$ versus $\log_{10}(E)$, where E is the error in the max norm for both $u_\epsilon - u_0$ and $u_\epsilon - u_0 - \epsilon\theta^*$. The slope α is the observed order of convergence $O(\epsilon^\alpha)$. The lines represent different boundary cutoffs δ, and the corresponding θ^* is different in each case. We also show the oscillatory error remaining after the first-order approximation in Figure 7.5. This would be corrected for by the addition of $\epsilon^2 u^{(2)}$.

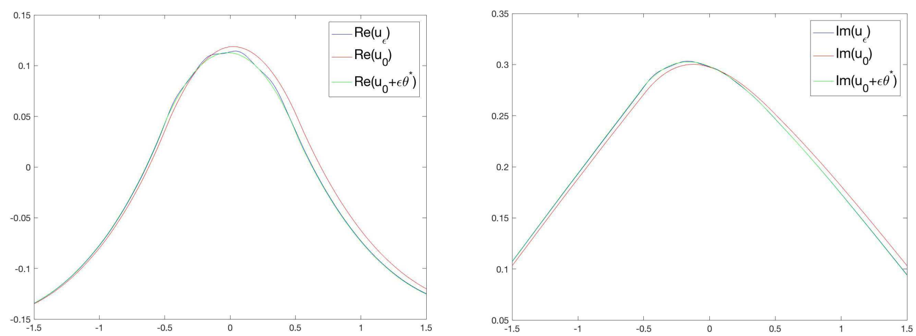

Fig. 7.1. *Square domain with smooth $n(y)$. $x_1 = 0$ slice of the solution versus first-order approximations assuming $\epsilon = 1/4$ and $k = 1$.*

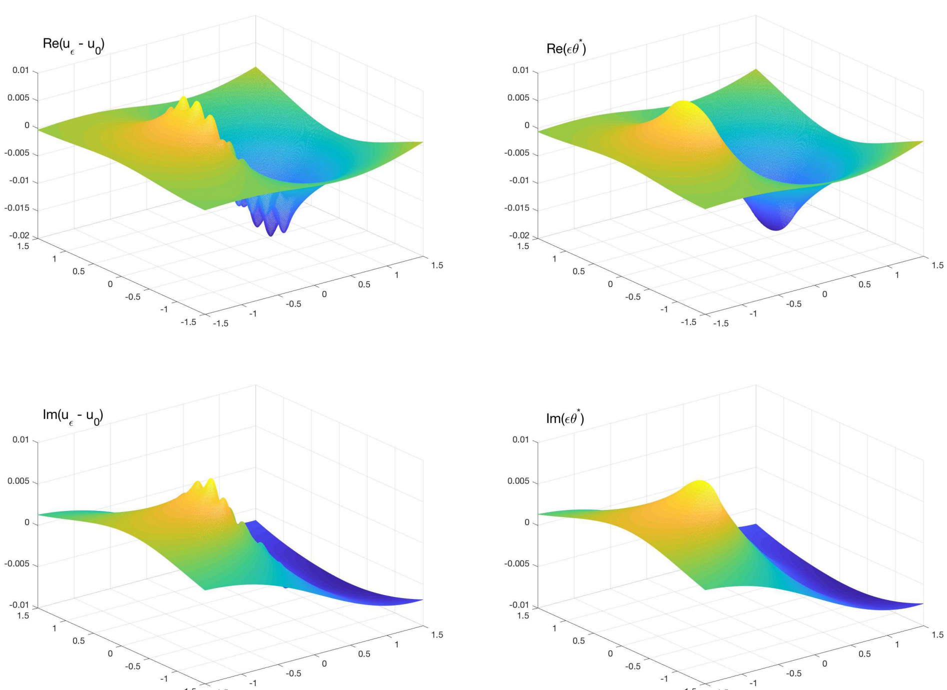

Fig. 7.2. *Square domain with smooth $n(y)$. Surface plots (real parts, top; imaginary parts, bottom) of $u_\epsilon - u_0$ (left) versus $\epsilon\theta^*$ (right) assuming $\epsilon = 1/4$ and $k = 1$.*

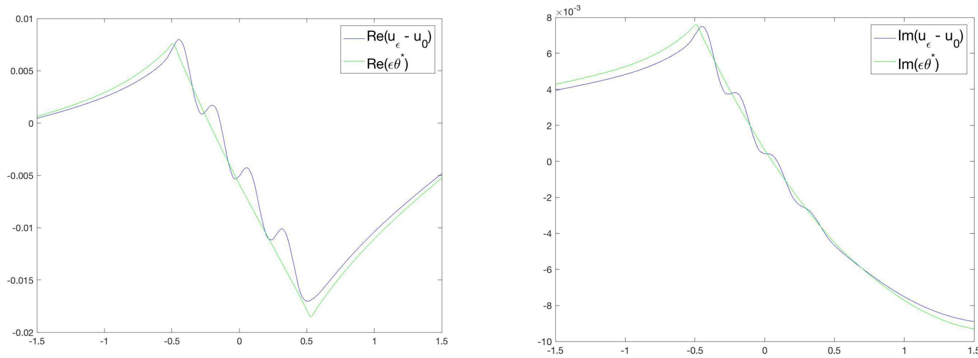

FIG. 7.3. *Square domain with smooth $n(y)$. $x_1 = 0$ slice of the first-order approximation residual versus the limiting boundary corrector $\epsilon\theta^*$ assuming $\epsilon = 1/4$ and $k = 1$: real parts (left) and imaginary parts (right).*

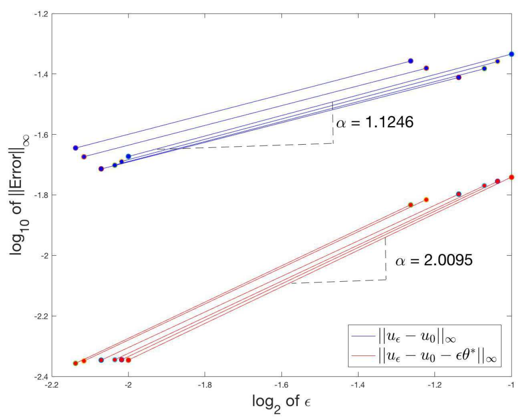

FIG. 7.4. *Square domain with smooth $n(y)$. Log-log plot showing the observed convergence ϵ^α: error without boundary correction (top cluster, blue) versus error with the limiting boundary correction $\epsilon\theta^*$ (bottom cluster, red). Individual lines correspond to different boundary cutoffs δ.*

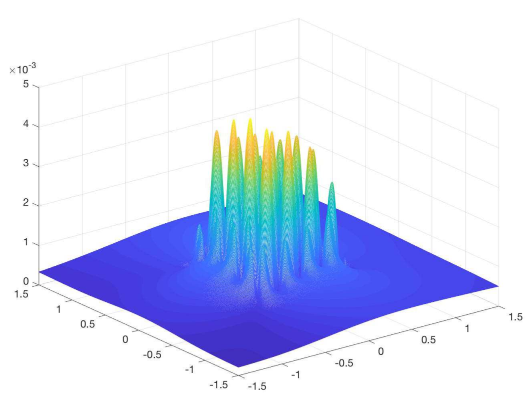

FIG. 7.5. *Square domain with smooth $n(y)$. Absolute error between u_ϵ and $u_0 + \epsilon\theta^*$ assuming $\epsilon = 1/4$ and $k = 1$.*

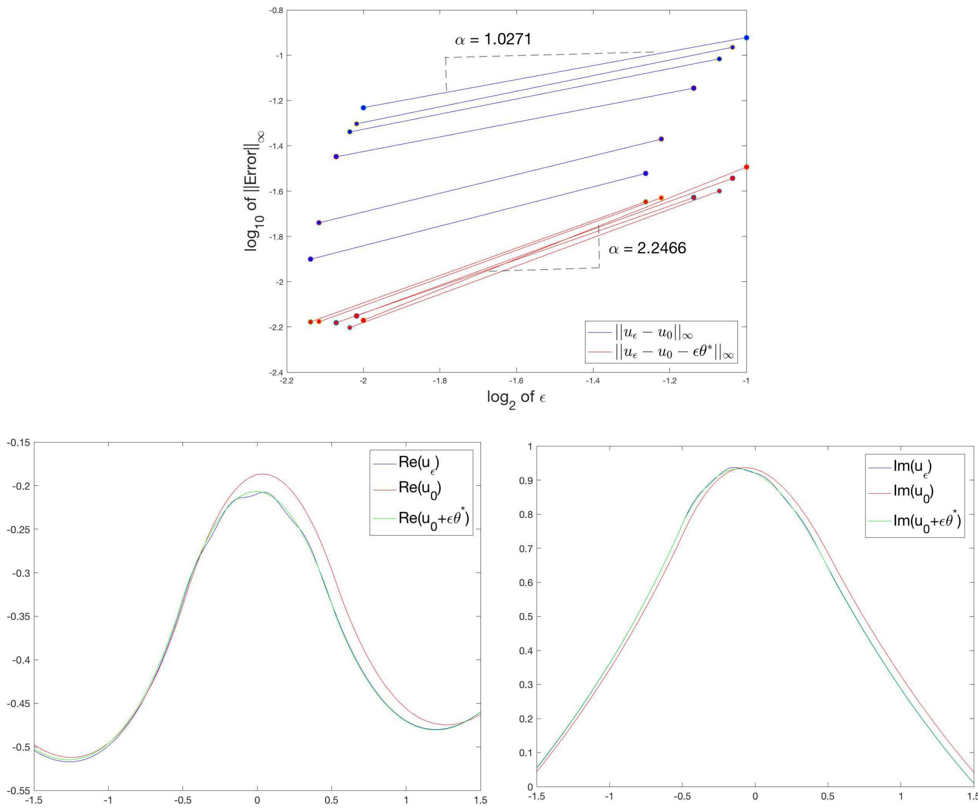

FIG. 7.6. *Square domain with layered $n(y)$. Top: log-log plot showing the observed convergence ϵ^α, error without boundary correction (top lines, blue) versus error with the limiting boundary correction $\epsilon\theta^*$ (bottom cluster, red). Individual lines correspond to different boundary cutoffs δ. Bottom: $x_1 = 0$ slices of u_ϵ, u_0 ad $u_0 + \epsilon\theta^*$ (real parts, left; imaginary parts, right) assuming $\epsilon = 1/4$ and $k = 1$.*

7.2. Piecewise-constant layering. In the next example, we choose a piecewise-constant periodic $n(y)$ given by the high-contrast variation

$$n(y) = \begin{cases} 6, & y_1 \in [0, 0.5), \\ 2, & y_1 \in [0.5, 1). \end{cases} \tag{7.1}$$

We can observe the convergence with and without the addition of θ^* in Figure 7.6. Again, the lines correspond to different boundary cutoffs δ. Note that with the addition of $\epsilon\theta^*$, which is different for each δ, we achieve an order of convergence of $O(\epsilon^2)$. For further illustration, we include pictures showing the effect of θ^* in Figure 7.7.

7.3. Circular domain. Let D be the circle centered at the origin with unit diameter endowed with

$$n(y) = 2 + \sin(2\pi y_1) + \cos(2\pi y_2).$$

As in the previous example, we can compute the scattered fields due to true and homogenized solutions on $\mathbb{R}^2$. Once again, let $a = I$ be the identity matrix. As stated in section 5.1, the limit θ^* is unique and in fact identically zero. However, $\|u_\epsilon - u_0\|$ is not in general $O(\epsilon^2)$, and we demonstrate this numerically. We compute

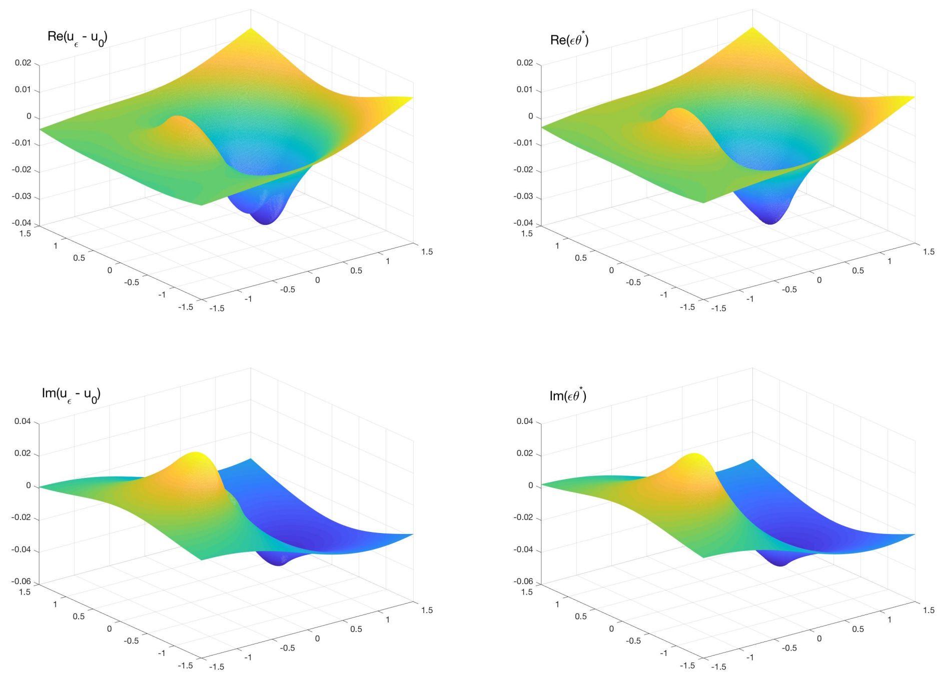

FIG. 7.7. *Square domain with layered $n(y)$. Surface plots (real parts, top; imaginary parts, bottom) of $u_\epsilon - u_0$ (left) and $\epsilon\theta^*$ (right) assuming $\epsilon = 1/4$ and $k = 1$.*

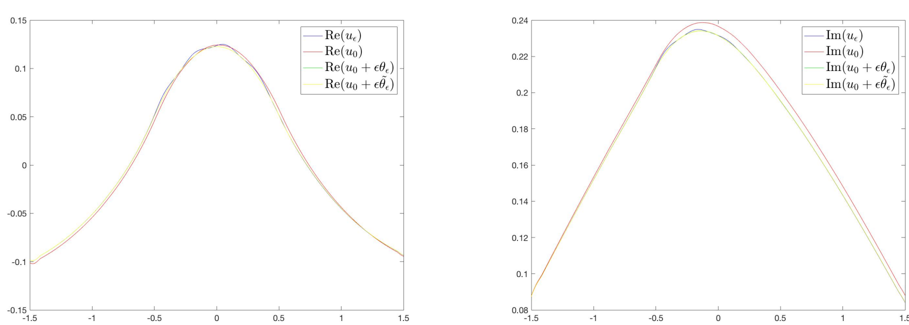

FIG. 7.8. *Circular domain with smooth $n(y)$. $x_1 = 0$ slices of u_ϵ (blue), u_0 (red), $u_0 + \epsilon\theta_\epsilon$ (green), and $u_0 + \epsilon\tilde{\theta}_\epsilon$ (yellow) assuming $\epsilon = 1/4$ and $k = 1$ (real parts, left; imaginary parts, right). Note that $\theta^* = 0$ so that $\tilde{\theta}_\epsilon$ correction is necessary to provide an $O(\epsilon^2)$ approximation.*

the boundary corrector θ_ϵ, the solution to (3.18), as well as the intermediary boundary corrector $\tilde{\theta}_\epsilon$, the solution to (5.3), to illustrate in detail their effects on the first-order approximation of the true solution.

Numerical results in Figures 7.8 and 7.9 show that without any boundary correction, we observe some differences between the brute force solution and its homogenized approximation that perpetuate outside of the circular scatterer. Both θ_ϵ and $\tilde{\theta}_\epsilon$ correct for this error in $u_\epsilon - u_0$. In Figure 7.10, we plot the convergence with and without the addition of a boundary corrector on a log-log scale. Note that with the addition of either $\epsilon\theta_\epsilon$ or $\epsilon\tilde{\theta}_\epsilon$ we achieve an $O(\epsilon^2)$ convergence, whereas without the correction we observe $u_\epsilon - u_0 = O(\epsilon^{3/2})$. As can be seen from Figure 7.11, the boundary corrector

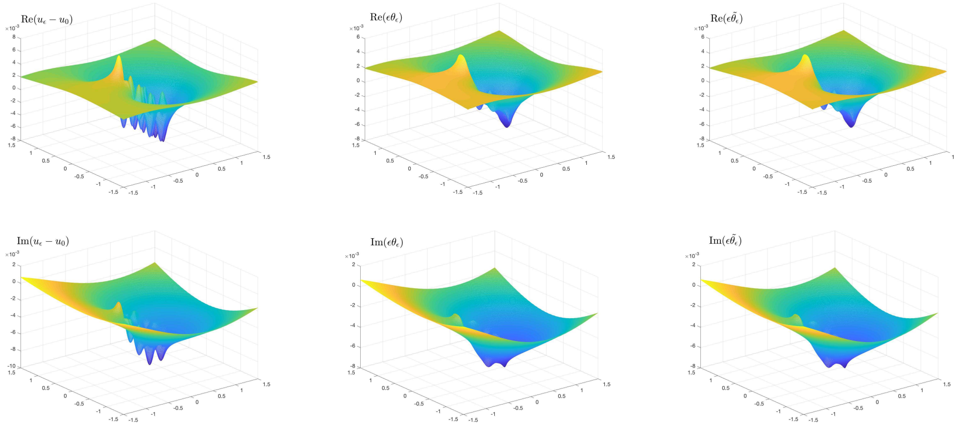

FIG. 7.9. *Circular domain with smooth $n(y)$. Real and imaginary parts of error $u_\epsilon - u_0$ (left), true boundary correction $\epsilon\theta_\epsilon$ (center), and approximate boundary correction $\epsilon\tilde{\theta}_\epsilon$ (right) assuming $\epsilon = 1/4$ and $k = 1$.*

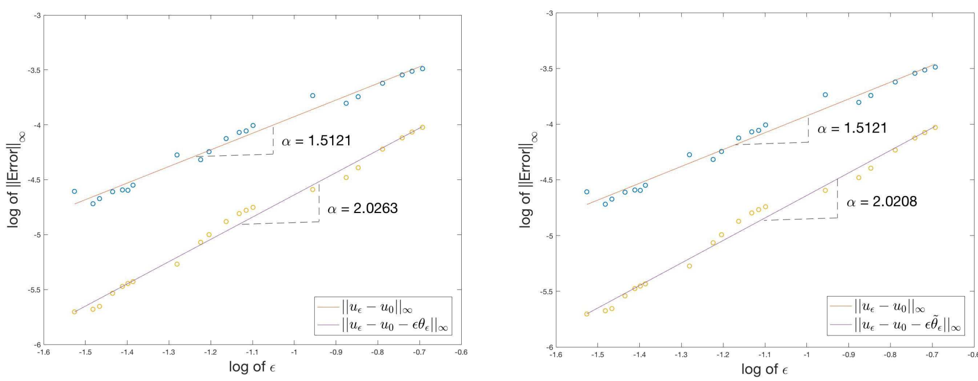

FIG. 7.10. *Circular domain with smooth $n(y)$. Log-log plot showing the observed ϵ^α convergence: error using θ_ϵ (left) versus error using $\tilde{\theta}_\epsilon$ (right). Note that in both cases the boundary correction improves the error rate from $O(\epsilon^{3/2})$ to $O(\epsilon^2)$.*

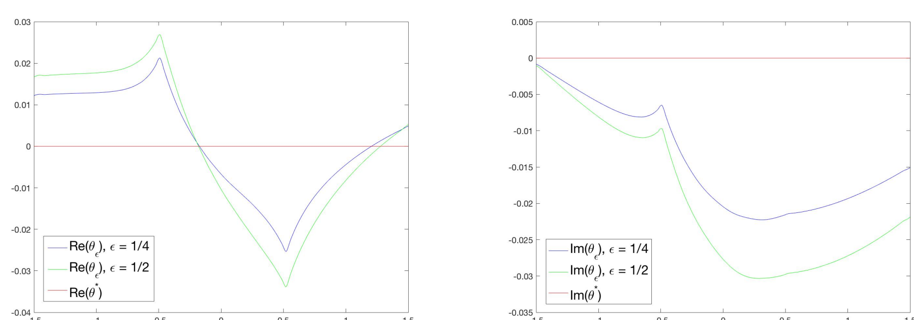

FIG. 7.11. *Circular domain with smooth $n(y)$. $x_1 = 0$ slices of the boundary corrector θ_ϵ assuming $k = 1$ and diminishing values od ϵ, illustrating the slow convergence to $\theta^* = 0$.*

θ_ϵ is converging to $\theta^* \equiv 0$. However, this convergence is relatively slow, and we see this in the observed orders of convergence of $u_\epsilon - u_0 \to 0$.

8. Conclusions. In this study, we establish a rigorous analysis of the boundary correction effects concerning two-scale approximation of the Helmholtz scattering by penetrable obstacles in $\mathbb{R}^d$ with periodically oscillating lower-order term. For this class of problems, we find that the boundary effects generally exist at all orders—and in fact constitute the leading-order correction of the homogenized solution. In the case of scatterers with piecewise-flat boundaries whose slopes are rational with respect to the axes of medium periodicity, we show that the limiting boundary corrector is nontrivial, permits explicit representation, and can be detected in the far field. For obstacles with smooth boundaries without flat parts, we further demonstrate that the boundary corrector converges to zero in the limit; however, this convergence is slow, and consequently the boundary effects still dominate the bulk correction. In this case, we propose to account for the boundary corrector by an effective model that features a homogenized interior coefficient but oscillating jump conditions. In terms of the affiliated inverse problem, we demonstrate that the first boundary correction is equivalent to the Born approximation of the scattered field due to periodic obstacle fluctuation about the mean index of refraction. We illustrate numerically the boundary correction effects for forward and inverse problems in $\mathbb{R}^1$ and those for the forward problems in $\mathbb{R}^2$ featuring either circular or square scatterer. The developments in this work naturally lend themselves to the analysis of nonperiodic microstructured media where $n = n(x, x/\epsilon)$, which is the subject of future work.

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