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Volume Integral Equation Methods for Scattering from Gratings: The TM Case

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Abstract

We analyze electromagnetic TM scattering from a diffraction grating consisting of a dielectric with possibly negative real part. The scattering problem can be reformulated as a strongly singular volume integral equation, a technique that attracts continuous interest in the engineering community, but rarely received rigorous theoretic treatment. In this paper, we provide (generalized) Gårding estimates in weighted and unweighted Sobolev spaces for the integral equation. Moreover, we show that trigonometric Galerkin methods applied to a periodization of the integral equation converge. Fully discrete formulas show that the numerical scheme is easy to implement and numerical examples show the performance of the method.

1 Introduction

We consider scattering of time-harmonic electromagnetic waves from diffraction gratings, three dimensional dielectrics that are periodic in one spatial direction and invariant in a second, orthogonal, direction. These optical components are used, e.g., to split up light into beams with different directions, and they serve in optical devices as, e.g., monochromators or as optical spectrometers.

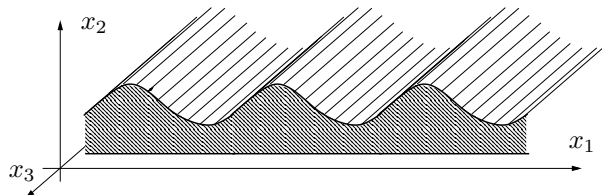


Figure 1: The setting for the scattering problem. The diffraction grating is periodic in x_1 , invariant in x_3 and bounded in x_2 .

If the wave vector of an incident electromagnetic plane wave is chosen perpendicular to the invariance direction of the grating, Maxwell's equations decouple into scalar Helmholtz equations, known as transverse magnetic (TM) and transverse electric (TE) modes (these terms are not consistently used in the literature). In this paper, we consider the equation of the TM mode for a non-magnetic grating,

$$\operatorname{div}(a\nabla u) + k^2 u = 0, \quad k > 0,$$

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under quasi-periodicity conditions for the field u . In particular, we allow the real part of the material parameter a to take negative values, a feature that arises for, e.g., optical negative-index metamaterials, but also for metals at certain frequencies. We use volume integral equations to obtain solution theory for the scattering problem, and we analyze the convergence of Galerkin methods based on trigonometric polynomials to discretize these integral equations.

In the engineering community, volume integral equations are a popular tool to numerically solve scattering problems, see, e.g., [9, 17, 26, 27], since they allow to solve problems with complicated material parameters via one single integral equation. The linear system resulting from the discretization of the integral operator (by, e.g., collocation or finite element methods) is large and dense. Still, the convolution structure of the integral operator allows to compute matrix-vector multiplications by FFT techniques in an order-optimal way (up to logarithmic terms), see, e.g., [24, 32, 34]. However, the discretization of the integral operator itself is sometimes done in a crude way, and a convergence analysis of the technique is often missing, in particular when material parameters are not globally smooth. For the problem that we investigate here, a particularly difficult situation occurs, because the occurring strongly singular integral operators are not compact (but the form of the integral equations is of the second kind).

Recently, volume integral equations also started to attract interest in the applied mathematics community. The papers [13, 14, 18, 33] provide numerical analysis for the Lippmann-Schwinger integral equation, when the integral operator is compact. Further, [7, 16, 23] analyze strongly singular integral equations for scattering in free space. However, [23] considers media with globally continuous material properties, and the L^2 -theory in [16] does not yield physical solutions if the material parameter appearing in the highest-order coefficients are not smooth. The paper [7] proves a Gårding inequality for a strongly singular volume integral equation arising from electromagnetic scattering from a (discontinuous) dielectric. This implies the convergence of Galerkin discretizations. However, setting up the full system matrix is costly both in terms of memory and CPU time. The strong singularity of the integral kernel even makes the computation of the diagonal of the system matrix challenging.

Our first aim in this paper is to analyze the quasiperiodic TM mode equation using volume integral equations, generalizing an approach from [16]. In [16], similar volume integral equations have been analyzed for free space scattering problems and positive contrast. In this paper, we prove Gårding inequalities in a (quasi-)periodic setting, and adapt the techniques from [16] to tackle complex-valued material parameters possibly having a negative real part. Some of our results also extend to anisotropic structures, and all results can be transferred to free space scattering problems. An important aspect of the analysis is that the dielectric properties of the medium are discontinuous at the air/grating interface (otherwise, the integral operators can be reduced to compact ones, see, e.g., [6, Chapter 9]).

Our second aim is to rigorously analyze a numerical method to solve the TM scattering problem by trigonometric Galerkin methods, again for discontinuous media. This technique originally stems from [33], where a corresponding collocation method for volume integral equations involving a compact integral operator has been analyzed. We prove that the trigonometric Galerkin method converges with optimal order, and give fully discrete formulas how to implement this method. Finally, we describe a couple of numerical experiments.

In essence, the advantage of the method is that it is simple to implement, and that the linear system can be evaluated at FFT speed. Of course, the convergence order is low if the medium has jumps, due to the use of global basis functions (if the material properties are globally smooth, then the method is high-order convergent). Nevertheless, the technique is an interesting tool for numerical simulation, as we demonstrate through numerical examples.

The analysis of the integral equation for material parameters with negative real part is, to the best of our knowledge, the first application of T -coercivity (see [2–4]) to volume integral equations.

The material parameter is, however, not allowed to take arbitrary negative values. The arising condition to guarantee solvability does for instance not allow the refractive index to take the value -1 inside the grating.

We would like to point out that the paper [4] analyzes Galerkin discretizations of variational formulations of Laplace-type problems with indefinite coefficients by using extension operators that map finite element spaces into itself. Our analysis is based on pretty similar extension operators, but clearly those do never map a space of trigonometric polynomials into itself. To this end, we provide an independent proof of that simple Galerkin methods applied to this problem converge, that might be useful for other problems, too (see Theorem 6.3).

The paper is organized as follows: In Section 2 we briefly recall variational theory for the direct scattering problem. In Sections 3 and 4 we introduce the corresponding integral equations and prove Gårding inequalities on a continuous level. In Sections 5 and 6 we prove Gårding inequalities for periodized integral equations, and error estimates for trigonometric Galerkin methods. Finally, Section 7 gives fully discrete formulas and two numerical examples. The two appendices contain two well-known results on differences of potential operators and extensions that do not fit comfortably into the main body of the text.

Notation: The usual L^2 -based Sobolev and Lipschitz spaces on a domain Ω are denoted as $H^s(\Omega)$ and $C^{n,1}(\overline{\Omega})$, respectively. Further, $H_{\text{loc}}^s(\Omega) = \{v \in H^s(B) \text{ for all open balls } B \subset \Omega\}$. The trace of a function u on ∂D from the outside and from the inside of D is $\gamma_{\text{ext}}(u)$ and $\gamma_{\text{int}}(u)$, respectively. The jump of u across ∂D is $[u]_{\partial D} = \gamma_{\text{ext}}(u) - \gamma_{\text{int}}(u)$. If the exterior and the interior trace of a function u coincide, we simply write $\gamma(u)$ for the trace.

2 Problem Setting

Propagation of time-harmonic electromagnetic waves in an inhomogeneous and isotropic medium without free currents is described by the time-harmonic Maxwell's equations for the electric and magnetic fields E and H , respectively,

$$\text{curl } H + i\omega\varepsilon E = \sigma E, \quad \text{curl } E - i\omega\mu_0 H = 0, \quad (1)$$

where $\omega > 0$ denotes the frequency, ε is the positive electric permittivity, μ_0 is the (constant and positive) magnetic permeability, and σ is the conductivity. We assume in this paper that all three scalar material parameters are independent of the third variable x_3 and 2π -periodic in the first variable x_1 . Further, ε equals $\varepsilon_0 > 0$ and σ equals zero outside the grating.

If an incident electromagnetic plane wave independent of the third variable x_3 illuminates the grating, then Maxwell's equations (1) for the total wave field decouple into two scalar partial differential equations (see, e.g., [22] or [8]). In particular, the third component H_3 of the magnetic field satisfies the two-dimensional scalar equation

$$\text{div} (\varepsilon_r^{-1} \nabla u) + k^2 u = 0 \quad \text{with } \varepsilon_r := \varepsilon_0^{-1}(\varepsilon + i\sigma/\omega) \text{ and } k := \omega\sqrt{\varepsilon_0\mu_0}, \quad (2)$$

together with jump conditions on interfaces where the refractive index ε_r^{-1} jumps: u and $\varepsilon_r^{-1} \partial u / \partial \nu$ are continuous across such interfaces. Note that ε_r is 2π -periodic in x_1 and equals one outside the grating. Working with weak solutions to (2), we assume that $\varepsilon_r \in L^\infty(\mathbb{R}^2, \mathbb{C})$ is such that $\varepsilon_r^{-1} \in L^\infty(\mathbb{R}^2, \mathbb{C})$ and $\text{Im}(\varepsilon_r) \leq 0$. Note that we do not assume that $\text{Re} \varepsilon_r^{-1} \geq c > 0$.

For the two-dimensional problem (2), incident electromagnetic waves reduce to $u^i(x) = \exp(ik \cdot x - d) = \exp(ik(x_1 d_1 + x_2 d_2))$ where $|d| = 1$ and $d_2 \neq 0$. When the incident plane wave u^i illuminates the diffraction grating there arises a scattered field u^s such that the total field $u = u^i + u^s$ satisfies (2). Since $\Delta u^i + k^2 u^i = 0$, the scattered field satisfies

$$\text{div} (\varepsilon_r^{-1} \nabla u^s) + k^2 u^s = -\text{div} (q \nabla u^i) \quad \text{in } \mathbb{R}^2, \quad (3)$$

where q is the contrast defined by

$$q = \varepsilon_r^{-1} - 1.$$

Note that u^i is α -quasi-periodic with respect x_1 , that is,

$$u^i(x_1 + 2\pi, x_2) = e^{2\pi i \alpha} u^i(x_1, x_2) \quad \text{for } \alpha := kd_1.$$

Since u^i is quasi-periodic and ε_r is periodic, the total field and the scattered field both are also quasi-periodic in x_1 . For uniqueness of solution, the scattered field has to satisfy a radiation condition. Here we require that u^s above (below) the dielectric structure can be represented by a uniformly converging Fourier(-Rayleigh) series consisting of upwards (downwards) propagating or evanescent plane waves, see [5, 15, 25],

$$u^s(x) = \sum_{j \in \mathbb{Z}} \hat{u}_j^\pm e^{i\alpha_j x_1 \pm i\beta_j(x_2 - \rho)}, \quad x_2 \gtrless \pm \rho, \quad \alpha_j = j + \alpha, \quad \beta_j = (k^2 - \alpha_j^2)^{1/2}, \quad (4)$$

where $\rho > \sup\{|x_2| : (x_1, x_2) \in \text{supp}(q)\}$. The numbers \hat{u}_j^\pm are the so-called Rayleigh coefficients of u^s , defined by $\hat{u}_j^\pm = (2\pi)^{-1} \int_{-\pi}^{\pi} u^s(x_1, \pm\rho) \exp(-i\alpha_j x_1) dx_1$. A solution to the Helmholtz equation is called radiating if it satisfies (4).

Variational solution theory for the scattering problem (3)–(4) is well-known, see [5, 8, 15], at least under the additional assumption that

$$k^2 \neq \alpha_j^2 \quad \text{for all } j \in \mathbb{Z}. \quad (5)$$

This assumption means that k^2 does not correspond to a Rayleigh-Wood frequency where the number of the propagating mode changes. Using Dirichlet-to-Neumann operators one can formulate the above scattering problem variationally in the bounded domain $\Omega_\rho := (-\pi, \pi) \times (-\rho, \rho)$, for $\rho > 0$ defined in (4), using the space $H_\alpha^1(\Omega_\rho) := \{u \in H^1(\Omega_\rho) : u = U|_{\Omega_\rho} \text{ for some } \alpha\text{-quasi-periodic } U \in H_{\text{loc}}^1(\mathbb{R}^2)\}$. For $s > 0$ and any set $X \subset \mathbb{R}^2$, the space $H_\alpha^s(X)$ of quasi-periodic functions in X is defined analogously. The variational formulation for the scattering problem (3, 4) is to find $u^s \in H_\alpha^1(\Omega_\rho)$ such that

$$\int_{\Omega_\rho} (\varepsilon_r^{-1} \nabla u^s \cdot \nabla \bar{v} - k^2 u^s \bar{v}) dx - \int_{\Gamma_\rho} \bar{v} T^+(u^s) ds - \int_{\Gamma_{-\rho}} \bar{v} T^-(u^s) ds = - \int_{\Omega_\rho} q \nabla u^i \cdot \nabla \bar{v} dx \quad (6)$$

for all $v \in H_\alpha^1(\Omega_\rho)$. The operators T^\pm , $\varphi \mapsto i \sum_{j \in \mathbb{Z}} \beta_j \hat{\varphi}_j^\pm e^{i\alpha_j x_1}$, are the so-called exterior Dirichlet-to-Neumann operators on Γ_\pm . The sesquilinear form in (6) is bounded on $H_\alpha^1(\Omega_\rho)$. It satisfies a Gårding inequality, if $\varepsilon_r^{-1} \geq c > 0$ in Ω_ρ .

In the latter case, Fredholm theory implies that existence of solution for problem (6) follows from uniqueness of solution. Existence of non-trivial solutions to the homogeneous problem where $u^i = 0$ in (6) is possible, but “rare”, since analytic Fredholm theory implies that the set of wave numbers in where non-uniqueness occurs is at most countable and has no accumulation point other than infinity, see [5, 10, 15]. If $\text{Re } \varepsilon_r^{-1}$ changes sign, Fredholm properties of the variational formulation (6) are non-trivial, at least if $\text{Im } \varepsilon_r^{-1}$ vanishes. For the above sesquilinear form, such properties do not seem to appear in the literature, however, [2–4] study corresponding Laplace-type problems with Dirichlet boundary conditions. Our analysis is rather based on a corresponding integral equation formulation.

3 Integral Equation Formulation

In this section, we reformulate the scattering problem (2) as a volume integral equation of the second kind and analyze this integral equation in weighted spaces. Here and in the rest of the

paper we assume the non-resonance condition (5). Let us denote by $\overline{D} \subset \Omega_\rho$ the support of the contrast $q = \varepsilon_r^{-1} - 1$, restricted to one period $\{-\pi < x_1 < \pi\}$. By $G_{k,\alpha}$ we denote the fundamental solution to the quasi-periodic Helmholtz equation in \mathbb{R}^2 . This function is well-defined for $x = (x_1, x_2)^\top$ with $x \neq (2\pi m, 0)^\top$ for $m \in \mathbb{Z}$,

$$G_{k,\alpha}(x) := \frac{i}{4\pi} \sum_{n \in \mathbb{Z}} \frac{1}{\beta_n} \exp(i\alpha_n x_1 + i\beta_n |x_2|), \quad (7)$$

see [19]. Since $k^2 \neq \alpha_n^2$ all the $\beta_n = (k^2 - \alpha_n^2)^{1/2}$ are non-zero. The following result from [15, pp. 90] will be useful in the sequel.

Lemma 3.1. *The Green's function $G_{k,\alpha}$ can be split into $G_{k,\alpha}(x) = (i/2)H_0^{(1)}(k|x|) + \Psi(x)$ in \mathbb{R}^2 where Ψ is an analytic function in that solves the homogeneous Helmholtz equation $\Delta\Psi + k^2\Psi = 0$ in $(-2\pi, 2\pi) \times \mathbb{R}$.*

Since we are interested in spectral schemes based on Fourier series, we also define a periodized Green's function by firstly setting

$$\mathcal{K}_\rho(x) := G_{k,\alpha}(x), \quad x = (x_1, x_2)^\top \in \mathbb{R} \times (-\rho, \rho), \quad x \neq (2\pi m, 0)^\top \text{ for } m \in \mathbb{Z}, \quad (8)$$

and secondly extending $\mathcal{K}_\rho(x)$ 2ρ -periodically in x_2 to \mathbb{R}^2 . The trigonometric polynomials

$$\varphi_j(x) := \frac{1}{\sqrt{4\pi\rho}} \exp\left(i\left[(j_1 + \alpha)x_1 + \frac{j_2\pi}{\rho}x_2\right]\right), \quad j = (j_1, j_2)^\top \in \mathbb{Z}^2, \quad (9)$$

are orthonormal in $L^2(\Omega_\rho)$. They differ from the usual Fourier basis (see, e.g., [29, Section 10.5.2]) only by a phase factor $\exp(i\alpha x_1)$, and hence also form a basis of $L^2(\Omega_\rho)$. For $f \in L^2(\Omega_\rho)$,

$$\hat{f}(j) := \int_{\Omega_\rho} f \overline{\varphi_j} dx, \quad j = (j_1, j_2)^\top \in \mathbb{Z}^2,$$

are the Fourier coefficients of f . For $0 \leq s < \infty$ we define a fractional Sobolev space $H_{\text{per}}^s(\Omega_\rho)$ as the subspace of functions in $L^2(\Omega_\rho)$ such that the norm $\|\cdot\|_{H_{\text{per}}^s(\Omega_\rho)}$,

$$\|f\|_{H_{\text{per}}^s(\Omega_\rho)}^2 = \sum_{j \in \mathbb{Z}^2} (1 + |j|^2)^s |\hat{f}(j)|^2 < \infty, \quad (10)$$

is finite. It is well-known that for integer values of s , these spaces correspond to spaces of (quasi-)periodic functions that are s times weakly differentiable, and that the above norm is then equivalent to the usual integral norms. Note that $H_{\text{per}}^s(\Omega_\rho) \subset H_\alpha^s(\Omega_\rho)$.

Lemma 3.1 implies in particular that \mathcal{K}_ρ has an integrable singularity, that is, the Fourier coefficients $\hat{\mathcal{K}}_\rho(j)$ are well-defined. For the next result, we set

$$\lambda_j := k^2 - (j_1 + \alpha)^2 - \left(\frac{j_2\pi}{\rho}\right)^2 \quad \text{for } j \in \mathbb{Z}^2.$$

If $\lambda \neq 0$, the following result is also contained in [28, Section 7.1].

Theorem 3.2. *Assume that $k^2 \neq \alpha_n^2$ for all $n \in \mathbb{Z}$. Then the Fourier coefficients of the kernel \mathcal{K}_ρ from (8) are given by*

$$\hat{\mathcal{K}}_\rho(j) = \begin{cases} \frac{\cos(j_2\pi)e^{i\beta j_1\rho} - 1}{\sqrt{4\pi\rho}\lambda_j} & \text{for } \lambda_j \neq 0, \\ \frac{i}{4j_2} \left(\frac{\rho}{\pi}\right)^{3/2} & \text{else,} \end{cases} \quad j = (j_1, j_2)^\top \in \mathbb{Z}^2.$$

Remark 3.3. $\hat{\mathcal{K}}_\rho(j)$ is well-defined for $\lambda_j = 0$: Since $k^2 \neq \alpha_n^2$ for all $n \in \mathbb{Z}$, the definition of λ_j implies that $j_2 \neq 0$ whenever $\lambda_j = 0$.

Proof. It is easy to check that $(\Delta + k^2)\varphi_j = \lambda_j\varphi_j$ for $j = (j_1, j_2)^\top \in \mathbb{Z}^2$. If $\lambda_j \neq 0$, Green's second identity implies that

$$\begin{aligned} \hat{\mathcal{K}}_\rho(j) &= \int_{\Omega_\rho} \mathcal{K}_\rho(x) \overline{\varphi_j(x)} \, dx = \lambda_j^{-1} \lim_{\delta \rightarrow 0} \int_{\Omega_\rho \setminus B(0, \delta)} G_{k, \alpha}(x) \overline{(\Delta + k^2)\varphi_j(x)} \, dx \\ &= \lambda_j^{-1} \lim_{\delta \rightarrow 0} \left[\left(\int_{\partial\Omega_\rho} + \int_{\partial B(0, \delta)} \right) \left(G_{k, \alpha} \frac{\partial \overline{\varphi_j}}{\partial \nu} - \frac{\partial G_{k, \alpha}}{\partial \nu} \overline{\varphi_j} \right) \, ds \right. \end{aligned} \quad (11)$$

$$\left. + \int_{\Omega_\rho \setminus B(0, \delta)} (\Delta + k^2) G_{k, \alpha}(x) \overline{\varphi_j(x)} \, dx \right], \quad (12)$$

where ν denotes the exterior normal vector to $B(0, \delta)$. The last volume integral vanishes since $(\Delta + k^2)G_{k, \alpha} = 0$ in $\Omega_\rho \setminus B(0, \delta)$ for any $\delta > 0$. Let us now consider the first integral in (11). The boundary of Ω_ρ consists of two horizontal lines $\Gamma_{\pm\rho}$ and two vertical lines $\{(x_1, x_2) : x_1 = \pm\pi, -\rho < x_2 < \rho\}$. Hence, the normal vector ν on these boundaries is either $(\pm 1, 0)^\top$ or $(0, \pm 1)^\top$. Straightforward computations yield that

$$G_{k, \alpha}(x_1, \pm\rho) = \frac{i}{4\pi} \sum_{n \in \mathbb{Z}} \frac{e^{i\beta_n \rho}}{\beta_n} e^{i\alpha_n x_1}, \quad \partial_2 G_{k, \alpha}(x_1, \pm\rho) = \mp \frac{1}{4\pi} \sum_{n \in \mathbb{Z}} e^{i\beta_n \rho} e^{i\alpha_n x_1}, \quad (13)$$

$$\overline{\varphi_j(x_1, \pm\rho)} = \frac{1}{\sqrt{4\pi\rho}} e^{-i\alpha_{j_1} x_1} \cos(j_2 \pi), \quad \text{and} \quad \partial_2 \overline{\varphi_j(x_1, \pm\rho)} = -\frac{ij_2 \pi}{\rho} \overline{\varphi_j(x_1, \pm\rho)}. \quad (14)$$

In consequence,

$$\begin{aligned} \int_{\Gamma_{\pm\rho}} \left(G_{k, \alpha} \frac{\partial \overline{\varphi_j}}{\partial \nu} - \frac{\partial G_{k, \alpha}}{\partial \nu} \overline{\varphi_j} \right) \, ds &= - \int_{\Gamma_\rho} \partial_2 G_{k, \alpha} \overline{\varphi_j} \, ds + \int_{\Gamma_{-\rho}} \partial_2 G_{k, \alpha} \overline{\varphi_j} \, ds \\ &= -2 \int_{\Gamma_\rho} \partial_2 G_{k, \alpha} \overline{\varphi_j} \, ds. \end{aligned}$$

Using the above formulae for $\partial_2 G_{k, \alpha}$ and $\overline{\varphi_j}$ in (13) and (14), respectively, we find that

$$-2 \int_{\Gamma_\rho} \partial_2 G_{k, \alpha} \overline{\varphi_j} \, ds = \frac{\cos(j_2 \pi)}{\sqrt{4\pi\rho}} \exp(i\beta_{j_1} \rho).$$

Computing the partial derivatives of $G_{k, \alpha}$ and φ_j with respect to x_1 analogously to the above computations, one finds that the integrals on the vertical boundaries of Ω_ρ vanish due to the α -quasi-periodicity of both functions. Thus, we obtain that

$$\int_{\partial\Omega_\rho} \left(G_{k, \alpha} \frac{\partial \overline{\varphi_j}}{\partial \nu} - \frac{\partial G_{k, \alpha}}{\partial \nu} \overline{\varphi_j} \right) \, ds = \frac{\cos(j_2 \pi)}{\sqrt{4\pi\rho}} \exp(i\beta_{j_1} \rho). \quad (15)$$

Now we consider the second integral in (11). From Lemma 3.1 we know that $G_{k, \alpha}(x) = \frac{i}{4} H_0^{(1)}(k|x|) + \Psi(x)$ where Ψ is a smooth function in Ω_ρ . Obviously,

$$\lim_{\delta \rightarrow 0} \int_{\partial B(0, \delta)} \left(\Psi \frac{\partial \overline{\varphi_j}}{\partial \nu} - \frac{\partial \Psi}{\partial \nu} \overline{\varphi_j} \right) \, ds = 0.$$

The asymptotics of $H_0^{(1)}$ and its derivative for small arguments,

$$H_0^{(1)}(r) = \frac{2i}{\pi} \log r + \mathcal{O}(1) \quad \text{and} \quad (H_0^{(1)})'(r) = \frac{2i}{\pi r} + \mathcal{O}(1) \quad \text{as } r \rightarrow 0,$$

allow to show that

$$\lim_{\delta \rightarrow 0} \int_{\partial B(0, \delta)} \left(G_{k, \alpha} \frac{\partial \overline{\varphi_j}}{\partial \nu} - \frac{\partial G_{k, \alpha}}{\partial r} \overline{\varphi_j} \right) ds = -\frac{1}{\sqrt{4\pi\rho}}, \quad (16)$$

see, e.g., [29, Theorem 2.2.1]. Combining (15) with (16) yields that

$$\mathcal{K}_\rho(j) = \frac{1}{\sqrt{4\pi\rho\lambda_j}} (\cos(j_2\pi) e^{i\beta_{j_1\rho}} - 1) \quad \text{for } \lambda_j \neq 0.$$

For $\lambda_j = 0$ we use de L'Hôpital's rule to find that

$$\mathcal{K}_\rho(j) = \lim_{\gamma \rightarrow (j_1 + \alpha)^2 + (j_2\pi/\rho)^2} \frac{\cos(j_2\pi) \exp(i\rho\sqrt{\gamma - (j_1 + \alpha)^2}) - 1}{\sqrt{4\pi\rho} [\gamma - (j_1 + \alpha)^2 - (j_2\pi/\rho)^2]} = \frac{i\rho^{3/2}}{4\pi^{3/2}j_2}.$$

□

Proposition 3.4. *Assume that $k^2 \neq \alpha_n^2$ for all $n \in \mathbb{Z}$. Then the convolution operator K_ρ , defined by*

$$(K_\rho f)(x) = \int_{\Omega_\rho} \mathcal{K}_\rho(x - y) f(y) dy \quad \text{for } x \in \Omega_\rho,$$

is bounded from $L^2(\Omega_\rho)$ into $H_{\text{per}}^2(\Omega_\rho)$.

Proof. Since $\varphi_j(x - z) = \sqrt{4\pi\rho} \varphi_j(x) \overline{\varphi_j(z)}$, we exploit the periodicity of $z \mapsto \mathcal{K}_\rho(z) \overline{\varphi_j(z)}$ to find that

$$\begin{aligned} (K_\rho \varphi_j)(x) &= \int_{\Omega_\rho} \mathcal{K}_\rho(x - y) \varphi_j(y) dy = \int_{x - \Omega_\rho} \mathcal{K}_\rho(z) \varphi_j(x - z) dz \\ &= \sqrt{4\pi\rho} \varphi_j(x) \int_{\Omega_\rho} \mathcal{K}_\rho(z) \overline{\varphi_j(z)} dz = \sqrt{4\pi\rho} \hat{\mathcal{K}}_\rho(j) \varphi_j(x). \end{aligned}$$

Let $f \in L^2(\Omega_\rho)$ with Fourier coefficients $\hat{f}(j)$ for $j \in \mathbb{Z}^2$, and set $f_N = \sum_{|j| \leq N} \hat{f}(j) \varphi_j$. Then

$$K_\rho f_N = \sum_{|j| \leq N} \hat{f}(j) K_\rho \varphi_j = \sqrt{4\pi\rho} \sum_{|j| \leq N} \hat{f}(j) \hat{\mathcal{K}}_\rho(j) \varphi_j$$

and

$$\|K_\rho f_N\|_{H_{\text{per}}^2(\Omega_{2\rho})}^2 \leq 4\sqrt{\pi\rho} \sum_{|j| \leq N} [1 + (j_1 + \alpha)^2 + (j_2\pi/\rho)^2]^2 |\hat{f}(j)|^2 |\hat{\mathcal{K}}_\rho(j)|^2.$$

From the computation of the coefficients $\hat{\mathcal{K}}_\rho(j)$ in Theorem 3.2 we know that there is $C = C(k)$ such that $|\hat{\mathcal{K}}_\rho(j)| \leq C/(1 + (j_1 + \alpha)^2 + (j_2\pi/\rho)^2)$. Hence $\|K_\rho f_N\|_{H_{\text{per}}^2(\Omega_{2\rho})} \leq C \|f_N\|_{L^2(\Omega_{2\rho})}$ for a constant C independent of $N \in \mathbb{N}$. Passing to the limit as $N \rightarrow \infty$ shows the claim of the proposition. □

Recall that $D \subset \Omega_\rho$ is the support of contrast q ; let us additionally introduce $\Omega := (-\pi, \pi) \times \mathbb{R}$.

Lemma 3.5. *Assume that $k^2 \neq \alpha_n^2$ for all $n \in \mathbb{Z}$. Then the volume potential V_k defined by*

$$(V_k f)(x) = \int_D G_{k,\alpha}(x-y)f(y) \, dy, \quad x \in \Omega,$$

is bounded from $L^2(D)$ into $H_\alpha^2(\Omega_R)$ for all $R > 0$.

Proof. Consider $\chi \in C^\infty(\Omega)$ such that $\chi = 1$ in D , $0 \leq \chi \leq 1$ in $\Omega_\rho \setminus \overline{D}$ and $\chi(x) = 0$ for $|x_2| > \rho$. Then $V_k g = \chi V_k g + (1-\chi)V_k g$. Note that $(1-\chi)V_k g = \int_D (1-\chi)G(\cdot-y)g(y) \, dy$ is an integral operator with a smooth kernel, since the series in (7) converges absolutely and uniformly for $|x_2| \geq \rho > 0$, as well as all its partial derivatives. The integral operator $(1-\chi)V_k$ is bounded from $L^2(D)$ into $H_\alpha^2(\Omega_R)$, since

$$\|\partial_1^{\beta_1} \partial_2^{\beta_2} ((1-\chi)V_k g)\|_{L^2(\Omega_R)}^2 \leq \int_{\Omega_R} \int_D |\partial_1^{\beta_1} \partial_2^{\beta_2} [(1-\chi(x))G_{k,\alpha}(x-y)]|^2 \, dy \, dx \, \|g\|_{L^2(D)}^2$$

for all $\beta_{1,2} \in \mathbb{N}$ such that $\beta_1 + \beta_2 \leq 2$.

It remains to show the boundedness of χV_k from $L^2(D)$ into $H^2(\Omega_\rho)$. Let $g \in L^2(D)$ and consider the operator $K_{2\rho}$ from Proposition 3.4, mapping $L^2(\Omega_{2\rho})$ into $H_{\text{per}}^2(\Omega_{2\rho}) \subset H_\alpha^2(\Omega_{2\rho})$,

$$(K_{2\rho} g)(x) = \int_D \mathcal{K}_{2\rho}(x-y)g(y) \, dy \quad \text{for } x \in \Omega_{2\rho}.$$

If $x \in \Omega_\rho$, then $|x_2 - y_2| \leq 2\rho$, that is, $\mathcal{K}_{2\rho}(x-y) = G_{k,\alpha}(x-y)$. Hence, $K_{2\rho} g = V_k g$ in Ω_ρ , and hence $\chi K_{2\rho} g = \chi V_k g$ in Ω_ρ . Since χ is a smooth function, we conclude that χV_k is bounded from $L^2(D)$ into $H_\alpha^2(\Omega_\rho)$. \square

Note that the potential $V_k f$ can be extended to a quasi-periodic function in $H_{\text{loc}}^2(\mathbb{R}^2)$, due to the quasi-periodicity of the kernel.

Lemma 3.6. *For $g \in L^2(D)^2$ the potential $w = \text{div } V_k g$ belongs to $H_\alpha^1(\Omega_\rho)$ for all $\rho > 0$. It is the unique radiating weak solution to $\Delta w + k^2 w = -\text{div } g$ in Ω , that is, it satisfies*

$$\int_\Omega (\nabla w \cdot \nabla \bar{v} - k^2 w \bar{v}) \, dx = - \int_D g \cdot \nabla \bar{v} \, dx \quad (17)$$

for all $v \in H_\alpha^1(\Omega)$ with compact support, and additionally the Rayleigh expansion condition (4).

Proof. Lemma 3.5 and quasi-periodicity of the kernel of V_k imply that w is a function in $H_\alpha^1(\Omega_\rho)$ for all $\rho > 0$. It is sufficient to prove (17) for all smooth quasi-periodic testfunctions v with compact support. It is also well-known that $p = L_k(g) \in H_\alpha^2(\Omega)$ is a weak solution to the Helmholtz equation, that is,

$$\int_\Omega (\nabla p_j \cdot \nabla \partial_j \bar{v} - k^2 p_j \partial_j \bar{v}) \, dx = - \int_D g_j \partial_j \bar{v} \, dx$$

for $j = 1, 2, 3$. An integration by parts shows that (note that no boundary terms arise, due to the choice of the testfunction)

$$\int_\Omega (\nabla \text{div } p \cdot \nabla \bar{v} - k^2 \text{div } p \bar{v}) \, dx = - \int_D g \cdot \nabla \bar{v} \, dx,$$

which implies (17) due to $\text{div } p = w$. Since the components of the potential $p = L_k(g)$ satisfy the Rayleigh condition, a simple computation shows that the divergence $w = \text{div } w$ does also satisfy the latter condition.

It remains to prove uniqueness of a radiating solution to (17) when g vanishes. Then w belongs to $H_\alpha^1(\Omega_\rho)$ for any $\rho > 0$ and satisfies the variational formulation (6) for $\varepsilon_r^{-1} = 1$ with right-hand side equal to zero. Choosing $v = u^s$ in (6) and taking the imaginary part of the equation shows that

$$\sum_{j: k^2 > \alpha_j^2} |k^2 - \alpha_j^2|^{1/2} (|\hat{u}_j^+|^2 + |\hat{u}_j^-|^2) = 0.$$

We conclude that all the propagating modes $\{j \in \mathbb{Z} : k^2 > \alpha_j^2\}$ vanish. Hence,

$$w(x) = \sum_{j: k^2 < \alpha_j^2} \hat{u}_j^\pm e^{i\alpha_j x_1 \mp |\alpha_j^2 - k^2|^{1/2}(x_2 - \rho)}, \quad x_2 \gtrless \pm \rho, \quad (18)$$

that is, w decays exponentially as $x_2 \rightarrow \pm\infty$. The unique continuation property for elliptic equations (see [21, Lemma 4.15] for a version that is applicable in our context) yields the equality

$$\int_{-\pi}^{\pi} w(x) e^{-i\alpha_j x_1} dx_1 = 2\pi \hat{u}_n^+ e^{|\alpha_j^2 - k^2|^{1/2}(x_2 - \rho)} =: w_n^+(x_2) \quad \text{for } x_2 \in \mathbb{R}.$$

Obviously, w_n^+ grows exponentially as $x_2 \rightarrow -\infty$ if and only if $\hat{u}_n^+ \neq 0$. Since w decreases exponentially as $x_2 \rightarrow -\infty$ due to (18), we conclude that all coefficients \hat{u}_n^+ vanish. Another application of the unique continuation property yields that w vanishes. \square

Let us now come back to the differential equation (3) for the scattered field u^s . If we set $f = q\nabla u^i$, then the variational formulation of (3) is

$$\int_{\Omega} (\nabla u^s \cdot \nabla \bar{v} - k^2 u^s \bar{v}) dx = - \int_D (q\nabla u^s + f) \cdot \nabla \bar{v} dx \quad (19)$$

for all $v \in H_\alpha^1(\Omega)$ with compact support in $\bar{\Omega}$. From Lemma 3.6 we know that the radiating solution to this problem is given by $v = \operatorname{div} V_k(q\nabla v + f)$. Hence, we aim to find a solution $v \in H_{\alpha, \text{loc}}^1(\Omega)$ to the integral equation

$$v - \operatorname{div} V_k(q\nabla v) = \operatorname{div} V_k(f) \quad \text{in } \Omega. \quad (20)$$

4 Gårding Inequalities

For scattering problems in free space, integral equations similar to (20) have been investigated in [16] for positive contrast q . In particular, this reference establishes a Gårding inequality for $I - \operatorname{div} V_k(q\nabla \cdot)$ in a weighted H^1 -space. In this section, we firstly apply a similar technique as in [16] to derive a Gårding inequality for $I - \operatorname{div} V_k(q\nabla \cdot)$ in a weighted quasi-periodic H^1 -space. Secondly, we extend this estimate to unweighted spaces, and we also treat material parameters with negative real (such that $\operatorname{Re}(q) < -2$).

From (20) it is obvious that the knowledge of u in D is sufficient to determine u in $\Omega \setminus \bar{D}$ by integration. Thus, we define the operator L_k by $L_k v = \operatorname{div} V_k v$ for $v \in L^2(D)$ and consider (20) restricted to D ,

$$u = L_k(q\nabla u + f) \quad \text{in } H_\alpha^1(D). \quad (21)$$

To study Gårding inequalities for volume integral equations, we introduce suitable weighted Sobolev spaces. An important assumption for the rest of the text is that the real part of the contrast does not vanish on D , $\operatorname{Re}(q) \neq 0$ on D . Then we denote by $H_{\alpha, q}^1(D)$ the completion of $H_\alpha^1(D)$ with respect to the norm $\|\cdot\|_{H_{\alpha, q}^1(D)}$, defined by

$$\|u\|_{H_{\alpha, q}^1(D)}^2 := \|\sqrt{|\operatorname{Re}(q)|} \nabla u\|_{L^2(D)}^2 + \|u\|_{L^2(D)}^2.$$

Note that $\|u\|_{H_{\alpha,q}^1(D)}$ is an equivalent norm in $H_{\alpha}^1(D)$ provided that $|\operatorname{Re}(q)|$ is bounded from below by some positive constant. In general,

$$\|u\|_{H_{\alpha,q}^1(D)} \leq (1 + \|\sqrt{|\operatorname{Re}(q)|}\|_{L^{\infty}(D)})\|u\|_{H_{\alpha}^1(D)}. \quad (22)$$

Note also that the norm of $H_{\alpha,q}^1(D)$ is linked to the sesquilinear form

$$a_q(u, v) = \int_D [\operatorname{sign}(\operatorname{Re}(q))q\nabla u \cdot \nabla \bar{v} + u\bar{v}] \, dx, \quad u, v \in H_{\alpha,q}^1(D). \quad (23)$$

Indeed, $\|u\|_{H_{\alpha,q}^1(D)}^2 = \operatorname{Re}[a_q(u, u)]$ for $u \in H_{\alpha,q}^1(D)$. Here, sesquilinear forms are, by definition, linear in the first argument and anti-linear in the second. The form a_q is also non-degenerate, and, if q is real, then a_q is simply the inner product associated with the norm of $H_{\alpha,q}^1(D)$,

$$\langle u, v \rangle_{H_{\alpha,q}^1(D)} = \int_D [q|\nabla u \cdot \nabla \bar{v} + u\bar{v}] \, dx, \quad u, v \in H_{\alpha,q}^1(D).$$

Lemma 4.1. *The operator $v \mapsto L_k(q\nabla v)$ is bounded from $H_{\alpha,q}^1(D)$ into itself.*

Proof. Due to Theorem 3.5, L_k is bounded from $L^2(D)^2$ into $H_{\alpha}^1(D)$. Furthermore, $v \mapsto q\nabla v$ is bounded from $H_{\alpha,q}^1(D)$ into $L^2(D)^2$, since

$$\|q\nabla v\|_{L^2(D)} \leq \|\sqrt{q}\|_{L^{\infty}(D)}\|v\|_{H_{\alpha,q}^1(D)}. \quad (24)$$

Moreover, the imbedding $H_{\alpha}^1(D) \subset H_{\alpha,q}^1(D)$ is bounded due to (22). Hence, $v \mapsto L_k(q\nabla v)$ is bounded on $H_{\alpha,q}^1(D)$. \square

If $u \in H_{\alpha}^1(D) \subset H_{\alpha,q}^1(D)$ solves the Lippmann-Schwinger equation (21), then Lemma (4.1) implies that u solves the same equation in $H_{\alpha,q}^1(D)$. Since a_q is non-degenerate, solving the Lippmann-Schwinger equation in $H_{\alpha,q}^1(D)$ is equivalent to solve

$$a_q(u - L_k(q\nabla u), v) = a_q(f, v) \quad \text{for all } v \in H_{\alpha,q}^1(D). \quad (25)$$

If $u \in H_{\alpha,q}^1(D)$ solves the latter variational problem for some $f \in H_{\alpha}^1(D)$, then $u = L_k(q\nabla u) + f$ belongs to $H_{\alpha}^1(D)$, due to (24) and since L_k is bounded from $L^2(D)$ into $H_{\alpha}^1(D)$.

Proposition 4.2. *Assume that $f \in H_{\alpha}^1(D)$. Then any solution to the Lippmann-Schwinger equation (21) in $H_{\alpha}^1(D)$ is a solution in $H_{\alpha,q}^1(D)$ and vice versa.*

Our aim is now first to prove a (generalized) Gårding inequality for the variational problem (25). Second, we use the latter result to derive a Gårding inequality for the original integral equation (21) in $H_{\alpha}^1(D)$. The following lemma will turn out to be useful.

Lemma 4.3. *Suppose that X and Y are Hilbert spaces. Let A, B be bounded linear operators from X into Y and consider the sesquilinear form $a : X \times X \rightarrow \mathbb{C}$, defined by $a(u, v) = \langle Au, Bv \rangle_Y$ for $u, v \in X$. If one of the operators A and B is compact, then the linear operator $Q : X \rightarrow X$, defined by $\langle Qu, v \rangle_X = a(u, v)$ for $u, v \in X$, is compact, too.*

Proof. It is easily seen that Q is a well-defined bounded linear operator. Obviously,

$$|\langle Qu, v \rangle_X| = |a(u, v)| \leq C\|Au\|_Y\|Bv\|_Y \quad \text{for } u, v \in X.$$

Assume that A is compact, and note that

$$\|Qu\|_X = \sup_{0 \neq v \in X} \frac{|\langle Qu, v \rangle_X|}{\|v\|_X} \leq C\|Au\|_Y.$$

If a sequence u_n converges weakly to zero in X , then Au_n contains a strongly convergent subsequence in Y . Consequently, Qu_n also contains a strongly convergent zero sequence. This in turn means that Q is compact. One can analogously derive the compactness of Q in case that B is compact, since $a(u, v) = \langle B^* Au, v \rangle$. \square

The next lemma shows Gårding inequalities for the operator $v \mapsto v - L_k(q\nabla v)$ using the sesquilinear form a_q from (23). The second part of the claim uses a periodic extension operator

$$E : H_\alpha^1(D) \rightarrow H_\alpha^1(\Omega), \quad E(u)|_D = u, \quad E(u)|_{\Omega \setminus \Omega_R} = 0,$$

introduced in Appendix B. The operator norm of E is

$$\|E\|_{H_\alpha^1(D) \rightarrow H_\alpha^1(\Omega_{2\rho})} = \left(1 + \|E\|_{H_\alpha^1(D) \rightarrow H_\alpha^1(\Omega_{2\rho} \setminus \overline{D})}^2\right)^{1/2}.$$

Theorem 4.4. (a) Assume that $\operatorname{Re}(q) > 0$ on D . Then there exists a compact operator K_+ on $H_{\alpha,q}^1(D)$ such that

$$\operatorname{Re} [a_q(v - L_k(q\nabla v), v)] \geq \|v\|_{H_{\alpha,q}^1(D)}^2 - \operatorname{Re} \langle K_+ v, v \rangle_{H_{\alpha,q}^1(D)}, \quad v \in H_{\alpha,q}^1(D). \quad (26)$$

(b) Assume that $\operatorname{Re}(q) < -1$, and that

$$\|E\|_{H_\alpha^1(D) \rightarrow H_\alpha^1(\Omega_{2\rho})} < \inf_D |\operatorname{Re}(q)|^{1/2}. \quad (27)$$

Then there exists a constant $C > 0$ and a compact operator K_- on $H_{\alpha,q}^1(D)$ such that

$$-\operatorname{Re} [a_q(v - L_k(q\nabla v), v)] \geq C \|v\|_{H_{\alpha,q}^1(D)}^2 - \operatorname{Re} \langle K_- v, v \rangle_{H_{\alpha,q}^1(D)}, \quad v \in H_{\alpha,q}^1(D). \quad (28)$$

Remark 4.5. If $\operatorname{Im}(q) = 0$ in D , then both statements (26) and (28) are nothing but standard Gårding estimates: The form a_q defines an inner product on $H_{\alpha,q}^1(D)$, and, e.g., (26) can be rewritten as $\operatorname{Re} \langle v - L_k(q\nabla v), v \rangle \geq \|v\|^2 - \operatorname{Re} \langle K_+ v, v \rangle$ for $v \in H_{\alpha,q}^1(D)$.

Proof. (a) We start with the case $\operatorname{Re}(q) > 0$ in D and prove that $I - L_i(q\nabla \cdot)$ is a coercive operator. Let $v \in H_{\alpha,q}^1(D)$ and define w by

$$w = L_i(q\nabla v) = \operatorname{div} \int_D G_{i,\alpha}(\cdot - y) q(y) \nabla v(y) \, dy \quad \text{in } \Omega. \quad (29)$$

Then $w \in H_\alpha^1(\Omega)$ decays exponentially to zero as $|x_2|$ tends to infinity. Moreover, $\Delta w - w = -\operatorname{div}(q\nabla v)$ holds in Ω in the weak sense due to Lemma 3.6, that is,

$$\int_\Omega [\nabla \psi^* \nabla w + \bar{\psi} w] \, dx = - \int_D q \nabla \psi^* \nabla v \, dx \quad \text{for all } \psi \in H_\alpha^1(\Omega). \quad (30)$$

Setting $\psi = w$, we find that $-\operatorname{Re} \int_D q \nabla w^* \nabla v \, dx = \|w\|_{H^1(\Omega)}^2$. Hence,

$$\begin{aligned} \operatorname{Re} [a_q(v - L_k(q\nabla v), v)] &= \operatorname{Re} \int_D [q|\nabla v|^2 + |v|^2 - q\nabla v^* \nabla w - w\bar{v}] \, dx \\ &= \int_D [\operatorname{Re}(q)|\nabla v|^2 + |v|^2 - \operatorname{Re}(w\bar{v})] \, dx + \int_\Omega [|\nabla w|^2 + |w|^2] \, dx \\ &\geq \|v\|_{H_{\alpha,q}^1(D)}^2 - \frac{1}{2} \|v\|_{L^2(D)}^2 + \frac{1}{2} \int_D \underbrace{[|v|^2 + |w|^2 - 2\operatorname{Re}(w\bar{v})]}_{=|v-w|^2} \, dx. \end{aligned}$$

In consequence,

$$\operatorname{Re} [a_q(v - L_k(q\nabla v), v)] \geq \|v\|_{H_{\alpha,q}^1(D)}^2 - \frac{1}{2}\langle v, v \rangle_{L^2(D)} - \operatorname{Re} \langle (L_k - L_i)v, v \rangle_{H_{\alpha,q}^1(D)}$$

for all $v \in H_{\alpha,q}^1(D)$. Due to Lemma 4.3 and the compact embedding of $H_{\alpha,q}^1(D)$ in $L^2(D)$, there exists a compact operator K_1 on $H_{\alpha,q}^1(D)$ such that

$$\frac{1}{2}\langle v, v \rangle_{L^2(D)} = \operatorname{Re} \langle K_1 v, v \rangle_{H_{\alpha,q}^1(D)}.$$

Further, the operator $K_2 := L_k - L_i$ is compact on $H_{\alpha}^1(D)$ due to the smoothness of the kernel shown in Appendix A. Hence K_2 is also compact on $H_{\alpha,q}^1(D)$ since the imbedding $H_{\alpha}^1(D) \subset H_{\alpha,q}^1(D)$ is bounded. Setting $K_+ := K_1 + K_2$, we obtain that

$$\operatorname{Re} \langle v - L_k(q\nabla v), v \rangle_{H_{\alpha,q}^1(D)} \geq \|v\|_{H_{\alpha,q}^1(D)}^2 - \operatorname{Re} \langle K_+ v, v \rangle_{H_{\alpha,q}^1(D)} \quad \text{for all } v \in H_{\alpha,q}^1(D).$$

(b) Now we consider the case that $\operatorname{Re}(q) < -1$, and assume additionally that (27) holds. As in the first part of the proof, we use the variational formulation (30) for w , defined as in (29), to find that

$$\begin{aligned} -\operatorname{Re} [a_q(v - L_k(q\nabla v), v)] &= \operatorname{Re} \int_D [q|\nabla v|^2 - |v|^2 - q\nabla v^* \nabla w + w\bar{v}] \, dx \\ &= \int_D [\operatorname{Re}(q)|\nabla v|^2 - |v|^2 + \operatorname{Re}(w\bar{v})] \, dx + \|w\|_{H_{\alpha}^1(\Omega)}^2 \\ &\geq \|w\|_{H_{\alpha}^1(\Omega)}^2 - \|v\|_{H_{\alpha,q}^1(D)}^2 - \operatorname{Re} \int_D w\bar{v} \, dx. \end{aligned}$$

We plug in $\psi = -E(v)$ into (30) and take the real part of that equation, to find that

$$\begin{aligned} \|\operatorname{Re} q|^{1/2} \nabla v\|_{L^2(D)}^2 &\leq \|w\|_{H_{\alpha}^1(\Omega)} \|E(v)\|_{H_{\alpha}^1(\Omega)} \leq \|E\|_{H_{\alpha}^1(D) \rightarrow H_{\alpha}^1(\Omega_{2\rho})} \|w\|_{H_{\alpha}^1(\Omega)} \|v\|_{H_{\alpha}^1(D)} \\ &\leq \|E\| \|w\|_{H_{\alpha}^1(\Omega)} \left(\|\operatorname{Re}(q)\|^{-1/2} \|v\|_{H_{\alpha,q}^1(D)} + \|v\|_{L^2(D)} \right). \end{aligned}$$

This implies that

$$\begin{aligned} \|v\|_{H_{\alpha,q}^1(D)}^2 - [1 + \|\operatorname{Re}(q)\|_{\infty}] \|v\|_{L^2(D)}^2 \\ \leq \|E\| \|\operatorname{Re}(q)\|^{-1/2} \|w\|_{H_{\alpha}^1(\Omega)} \left(\|v\|_{H_{\alpha,q}^1(D)} + \|\operatorname{Re}(q)\|^{1/2} \|v\|_{L^2(D)} \right). \end{aligned}$$

Rewriting the right-hand side of the latter inequality using the binomial theorem, and dividing by the term in brackets on the right, we obtain that

$$\|v\|_{H_{\alpha,q}^1(D)} - [1 + \|\operatorname{Re}(q)\|_{\infty}]^{1/2} \|v\|_{L^2(D)} \leq \|E\| \|\operatorname{Re}(q)\|^{-1/2} \|w\|_{H_{\alpha}^1(\Omega)}. \quad (31)$$

Note that the constant

$$\lambda_1 := \|E\|_{H_{\alpha}^1(D) \rightarrow H_{\alpha}^1(\Omega_{2\rho})} \|\operatorname{Re}(q)\|^{-1/2} \|w\|_{L^{\infty}(D)}$$

is, by assumption (27), less than one. If we set, for a moment, $C = [1 + \|\operatorname{Re}(q)\|_{\infty}]^{1/2}$, then (31) and Cauchy's inequality imply that

$$\begin{aligned} \lambda_1^2 \|w\|_{H_{\alpha}^1(\Omega)}^2 &\geq \|v\|_{H_{\alpha,q}^1(D)}^2 + C^2 \|v\|_{L^2(D)}^2 - 2C \|v\|_{H_{\alpha,q}^1(D)} \|v\|_{L^2(D)} \\ &\geq (1 - \varepsilon^2) \|v\|_{H_{\alpha,q}^1(D)}^2 + C^2 (1 - 1/\varepsilon^2) \|v\|_{L^2(D)}^2, \quad \varepsilon \in (0, 1). \end{aligned}$$

In consequence,

$$\begin{aligned}
-\operatorname{Re} [a_q(v - L_k(q\nabla v), v)] &\geq \left(\frac{1 - \varepsilon^2}{\lambda_1^2} - 1 \right) \|v\|_{H_{\alpha,q}^1(D)}^2 \\
&\quad - \operatorname{Re} \int_D w \bar{v} \, dx - C^2(1 - 1/\varepsilon^2) \|v\|_{L^2(D)}^2, \quad \varepsilon \in (0, 1). \quad (32)
\end{aligned}$$

Since $\lambda_1 < 1$ there exists $\varepsilon \in (0, 1)$ such that $1 - \varepsilon^2 > \lambda_1^2$, that is, $(1 - \varepsilon^2)/\lambda_1^2 - 1 > 0$. The last two terms on the right-hand side of (32) can be treated as compact perturbations just as in part (a) of this proof. \square

Remark 4.6. *All results so far can be extended to an anisotropic contrast $Q : \Omega \rightarrow \mathbb{C}^{2 \times 2}$ such that $\operatorname{Re} Q = (Q + Q^*)/2$ is a symmetric matrix-valued function a.e. in D , and such that the absolute value $\operatorname{Re} Q$ is either positive or negative definite in D (which determines the sign $\operatorname{sign}(\operatorname{Re} Q)$ of $\operatorname{Re} Q$). The term $\|\sqrt{|\operatorname{Re} Q|} \nabla u\|$ in the definition of $H_{\alpha,q}^1$ has to be replaced by $\|(\nabla u)^\top (\operatorname{sign}(\operatorname{Re} Q) \operatorname{Re} Q)^{1/2} \nabla u\|$, and the corresponding term in the definition of a_q has to be replaced by $\operatorname{sign}(\operatorname{Re} Q) (\nabla u)^\top Q \nabla \bar{v}$.*

For scalar q , the generalized Gårding inequalities from the last theorem can be transformed to estimates in the unweighted space $H_\alpha^1(D)$ using the following lemma.

Lemma 4.7. *Assume that D is a domain of class $C^{2,1}$ and that $\mu \in C_\alpha^{2,1}(\overline{D})$. Then*

$$T : H_\alpha^1(D) \rightarrow H_\alpha^1(D), \quad Tv := \operatorname{div} [\mu V_k(q\nabla(v/\mu)) - V_k(q\nabla v)],$$

is a compact operator.

Proof. We denote by $\mu^* \in C_\alpha^{2,1}(\overline{\Omega_\rho})$ an extension of $\mu \in C_\alpha^{2,1}(\overline{D})$ to Ω_ρ (see Appendix B on periodic extension operators). Then $\mu^*|_D = \mu$. Consider the two quasi-periodic functions

$$w_1 = \mu^* V_k(q\nabla(v/\mu)) \quad \text{and} \quad w_2 = V_k(q\nabla v) \quad \text{in } \Omega_\rho.$$

Both functions satisfy differential equations,

$$\Delta w_1 + k^2 w_1 = \begin{cases} -q\mu \nabla(v/\mu) + 2\nabla\mu \cdot \nabla w_1 + w_1 \Delta\mu & \text{in } D, \\ 2\nabla\mu^* \cdot \nabla w_1 + w_1 \Delta\mu^* & \text{in } \Omega_\rho \setminus \overline{D}, \end{cases}$$

and $\Delta w_2 + k^2 w_2 = -q\nabla v$ in D and $\Delta w_2 + k^2 w_2 = 0$ in $\Omega_\rho \setminus \overline{D}$. Hence, $w = w_1 - w_2$ solves

$$\Delta w + k^2 w = \begin{cases} -q\mu \nabla(1/\mu)v + 2\nabla\mu \cdot \nabla w_1 + w_1 \Delta\mu =: g_1 & \text{in } D, \\ w_1 \Delta\mu^* + 2\nabla\mu^* \cdot \nabla w_1 =: g_2 & \text{in } \Omega_\rho \setminus \overline{D}, \end{cases}$$

The functions g_1 and g_2 belong to $H_\alpha^1(D)$ and $H_\alpha^1(\Omega_\rho \setminus \overline{D})$, respectively. Their norms in these spaces are bounded by the norm of μ in $C_\alpha^{1,1}(\overline{D})$ times the norm of v in $H_\alpha^1(D)$. Due to Lemma 3.5, the jump of the trace and the normal trace of $w_{1,2}$ across ∂D vanishes. Hence, the Cauchy data of w are also continuous across the boundary of D .

Since the volume potential V_k is bounded from $L^2(D)$ into $H_\alpha^2(D)$, it is clear that w belongs to $H_\alpha^2(D)$. Moreover, we are now in a position where we can apply elliptic transmission regularity results [20, Theorem 4.20] to conclude that w is even smoother than H^2 . These regularity results will in turn imply the compactness of the operator $T : v \mapsto \operatorname{div} w$ on $H_\alpha^1(D)$. (Note that this step

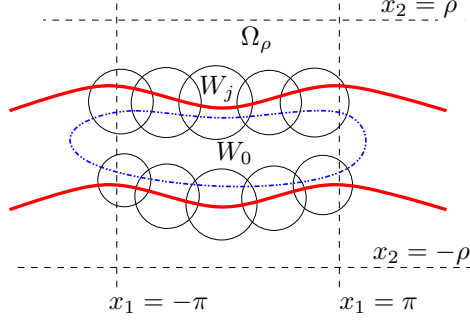


Figure 2: The sets W_j cover the domain D (one period of the support of the contrast q). These sets are used in the proof of Theorem 4.7.

requires the smoothness assumptions on D and μ .) Since [20, Theorem 4.20] is formulated for a bounded domain, we briefly mention how to extend this result to the periodic setting.

First, we extend w by periodicity to $\Omega'_\rho := (-3\pi, 3\pi) \times (-\rho, \rho)$ and proceed analogously with $g_{1,2}$. Then we choose a finite open cover $\{W_j\}_{j=1}^J$ consisting of smooth domains $W_j \subset \Omega'_\rho$ such that $\partial D \cap \Omega \subset \bigcup_{j=1}^J W_j$. In these smooth domains, we can then apply [20, Theorem 4.20] to obtain that

$$\|w\|_{H^3(W_j)} \leq C \left[\|w\|_{H^1_\alpha(\Omega_\rho)} + \|g_1\|_{H^1_\alpha(D)} + \|g_2\|_{H^1_\alpha(\Omega_\rho \setminus \overline{D})} \right].$$

Combining this estimate with an interior regularity result (e.g., [20, Theorem 4.18]) in a set W_0 such that $\overline{D} \subset \bigcup_{j=0}^J W_j$ (see Figure 2), we finally obtain that

$$\|w\|_{H^3(D)} \leq C \left[\|w\|_{H^1(\Omega_\rho)} + \|g_1\|_{H^1(D)} + \|g_2\|_{H^1(\Omega_\rho \setminus \overline{D})} \right] \leq C \|v\|_{H^1_\alpha(D)}.$$

□

The following lemma shows that the Gårding estimates in the weighted spaces $H^1_{\alpha,q}(D)$ can be transformed into estimates in $H^1_\alpha(D)$ if, roughly speaking, the real-valued contrast q is smooth enough and if $(\nabla q)/q$ is bounded.

Theorem 4.8. *Assume that the contrast q is real-valued, that $|q| \geq q_0 > 0$ in D , and that $\sqrt{|q|} \in C^{1,1}(\overline{D})$. Moreover, assume that D is of class $C^{2,1}$.*

(a) *For positive $q > 0$ there exists a compact operator K_+ on $H^1_\alpha(D)$ such that*

$$\operatorname{Re} \langle v - L_k(q\nabla v), v \rangle_{H^1_\alpha(D)} \geq \|v\|_{H^1_\alpha(D)}^2 - \operatorname{Re} \langle K_+ v, v \rangle_{H^1_\alpha(D)}, \quad v \in H^1_\alpha(D).$$

(b) *If $q < 0$ and if (27) holds, then there exists a compact operator K_- on $H^1_\alpha(D)$ such that*

$$-\operatorname{Re} \langle v - L_k(q\nabla v), v \rangle_{H^1_\alpha(D)} \geq C \|v\|_{H^1_\alpha(D)}^2 - \operatorname{Re} \langle K_- v, v \rangle_{H^1_\alpha(D)}, \quad v \in H^1_\alpha(D),$$

where C is the constant from (28).

Proof. We only prove case (a) here, supposing that $q > q_0 > 0$ in D . The proof for case (b) is analogous, essentially one needs to replace \sqrt{q} by $\sqrt{|q|}$. For simplicity, let us from now on abbreviate

$$\mu := \sqrt{q} \in C^{1,1}(\overline{D}).$$

Choose an arbitrary $u \in H_\alpha^1(D)$ and consider $v = u/\mu$. Our assumptions on q imply that $v \in H_{\alpha,q}^1(D)$, since

$$\|v\|_{H_{\alpha,q}^1(D)}^2 \leq (2 + \|1/\mu\|_\infty^2 + 2\|(\nabla\mu)/\mu\|_\infty^2)\|u\|_{H_\alpha^1(D)}^2.$$

In Theorem 4.4(a) (see also Remark 4.5) we showed that

$$\operatorname{Re} \langle v - L_k(q\nabla v), v \rangle_{H_{\alpha,q}^1(D)} \geq \|v\|_{H_{\alpha,q}^1(D)}^2 - \operatorname{Re} \langle K_1 v, v \rangle_{H_{\alpha,q}^1(D)},$$

where K_1 is a compact operator on $H_{\alpha,q}^1(D)$. This implies that

$$\begin{aligned} \operatorname{Re} \langle u - L_k(q\nabla u), u \rangle_{H_\alpha^1(D)} &\geq \|u\|_{H_\alpha^1(D)}^2 + \operatorname{Re} \langle K_1(u/\mu), u/\mu \rangle_{H_{\alpha,q}^1(D)} \\ &\quad + \operatorname{Re} \langle K_2 u, \nabla u \rangle_{L^2(D)} + \operatorname{Re} \langle K_3 u, u \rangle_{L^2(D)}, \end{aligned}$$

where

$$K_2 u = \nabla \left[\operatorname{div} [\mu V_k(q\nabla(u/\mu)) - V_k(q\nabla u)] \right] - \nabla \left[\nabla\mu \cdot V_k(q\nabla(u/\mu)) \right] + (\nabla\mu)L_k(q\nabla(u/\mu)),$$

$$\text{and } K_3 u = q\nabla(1/\mu) \cdot [\nabla L_k(q\nabla(u/\mu))] + L_k(q\nabla(u/\mu))/\mu - L_k(q\nabla u).$$

Lemma 4.7 shows that first term in the first line of the last equation yields a compact operator from $H_\alpha^1(D)$ into $L^2(D)$. The boundedness of the potentials V_k from $L^2(D)$ into $H_\alpha^2(D)$ and of L_k from $L^2(D)^2$ into $H_\alpha^1(D)$, and the smoothness of μ , allows to conclude that $K_2 : H_\alpha^1(D) \rightarrow L^2(D)$ is a compact operator and $K_3 : H_\alpha^1(D) \rightarrow L^2(D)$ is a bounded operator. Hence, Lemma 4.3 implies the existence of a compact operator K_+ on $H_\alpha^1(D)$ such that

$$\langle K_+ u, v \rangle_{H_\alpha^1(D)} = \operatorname{Re} \langle K_1(u/\mu), v/\mu \rangle_{H_{\alpha,q}^1(D)} + \operatorname{Re} \langle K_2 u, \nabla v \rangle_{L^2(D)} + \operatorname{Re} \langle K_3 u, v \rangle_{L^2(D)}$$

for $u, v \in H_\alpha^1(D)$, which proves the claim. \square

Remark 4.9. *The regularity assumptions on ∂D can be lowered using regularity theory for corner domains. Here we merely use the results and assumptions of [20, Theorem 4.18] to avoid technicalities.*

5 Periodization of the Integral Equation

In this section we reformulate the volume integral equation

$$u = L_k(q\nabla u + f) \quad \text{in } H_\alpha^1(D) \tag{33}$$

in a periodic setting and show the equivalence of the periodized equation and the original one. The purpose of this periodization, first introduced by Vainikko [33], is that the resulting integral operator is, roughly speaking, diagonalized by trigonometric polynomials. Fast FFT-based schemes become available to discretize the periodized integral operator and iterative schemes can be used to solve the corresponding operator equations. To establish convergence rates for these schemes, it is crucial to establish Gårding inequalities for the periodized integral operator.

For our purpose we additionally need to smoothen the kernel before periodizing. For $R > 2\rho$ we choose a function $\chi \in C^3(\mathbb{R})$ that is $2R$ -periodic, that satisfies $0 \leq \chi \leq 1$ and $\chi(x_2) = 1$ for $|x_2| \leq 2\rho$, and such that $\chi(R)$ vanishes up to order three, $\chi^{(j)}(R) = 0$ for $j = 1, 2, 3$ (compare Figure 3) Let us define a smoothed kernel \mathcal{K}_{sm} by

$$\mathcal{K}_{\text{sm}}(x) = \chi(x_2)\mathcal{K}_R(x) \quad \text{for } x \in \mathbb{R}^2, \quad x \neq [2\pi m, 2Rn]^\top, \quad m, n \in \mathbb{Z}, \tag{34}$$

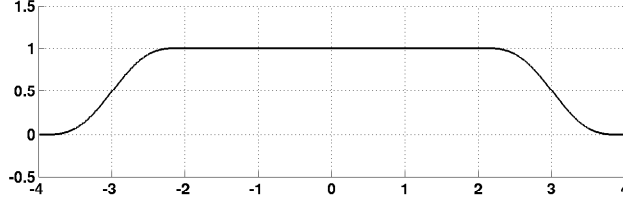


Figure 3: One period of the function χ is smooth, it equals one for $|x_2| \leq 2\rho$, and it vanishes at $\pm(R)$ up to order three. In this sketch, $\rho = 1$ and $R = 4$.

where \mathcal{K}_R is the kernel from (8). Note that \mathcal{K}_{sm} is α -quasi-periodic in x_1 , $2R$ -periodic in x_2 , and a smooth function on its domain of definition (that is, away from the singularities). We recall the trigonometric orthonormal basis of $L^2(\Omega_R)$ from (9),

$$\varphi_j(x) = (4\pi R)^{-1/2} \exp\left(i(j_1 + \alpha)x_1 + i\frac{j_2\pi}{R}x_2\right), \quad j = (j_1, j_2)^\top \in \mathbb{Z}^2, \quad (35)$$

and the associated Sobolev spaces $H_{\text{per}}^s(\Omega_R)$ from (10).

Lemma 5.1. *The integral operator $L_{\text{per}} : L^2(\Omega_R)^2 \rightarrow H_{\text{per}}^1(\Omega_R)$ defined by $L_{\text{per}}f = \text{div} \int_D \mathcal{K}_{\text{sm}}(\cdot - y)f(y) dy$ is bounded.*

Proof. We split the integral operator in two parts,

$$\begin{aligned} L_{\text{per}}f &= \text{div} \int_D \mathcal{K}_{\text{sm}}(\cdot - y)f(y) dy = \text{div} \int_D \chi(\cdot - y_2)\mathcal{K}_R(\cdot - y)f(y) dy \\ &= \text{div} \int_D \mathcal{K}_R(\cdot - y)f(y) dy + \text{div} \int_D [\chi(\cdot - y_2) - 1]\mathcal{K}_R(\cdot - y)f(y) dy. \end{aligned}$$

By Theorem 3.4, the integral operator with the kernel \mathcal{K}_R is bounded from $L^2(\Omega_R)^2$ into $H_\alpha^1(\Omega_R)$. Further, the definition of χ shows that $\chi(x_2 - y_2) - 1 = 0$ for $|x_2| \leq \rho$ and $y \in D$. The kernel $(\chi - 1)\mathcal{K}_R$ is hence smooth in Ω_R , and the corresponding integral operator is compact from $L^2(\Omega_R)^2$ into $H_\alpha^1(\Omega_R)$. Hence, L_{per} is bounded from $L^2(\Omega_R)^2$ into $H_\alpha^1(\Omega_R)$. The periodicity of the kernel \mathcal{K}_{sm} in the second argument finally implies that $L_{\text{per}}f$ belongs to $H_{\text{per}}^1(\Omega_R) \subset H_\alpha^1(\Omega_R)$. \square

Let us now consider the periodized integral equation

$$u - L_{\text{per}}(q\nabla u) = L_{\text{per}}(f) \quad \text{in } H_{\text{per}}^1(\Omega_R). \quad (36)$$

Theorem 5.2. (a) *If $f \in L^2(\Omega_R)^2$ is supported in \overline{D} , then $L_{\text{per}}(f)$ is equal to $L_k(f)$ in Ω_ρ .*

(b) *Problem (33) is uniquely solvable in $H_\alpha^1(D)$ for any right-hand side $f \in L^2(D)^2$ if and only if (36) is uniquely solvable in $H_{\text{per}}^1(\Omega_R)$ for any right-hand side $f \in L^2(\Omega_R)^2$ such that $\text{supp}(f) \subset \overline{D}$.*

(c) *If $q \in C^{1,1}(\overline{D})$ and if $f = q\nabla u^i$ for a smooth α -quasiperiodic function u^i , then any solution to (36) belongs to $H_{\text{per}}^s(\Omega_R)$ for $s < 3/2$.*

Proof. (a) For all x and $y \in \Omega_R$ such that $|x_2 - y_2| \leq 2\rho$ it holds that $\mathcal{K}_{\text{sm}}(x - y) = \chi(x_2 - y_2)\mathcal{K}_R(x - y) = G_{k,\alpha}(x - y)$. In particular, for $x \in \Omega_\rho$ and $y \in D \subset \Omega_\rho$ it holds that $|x_2 - y_2| \leq 2\rho$.

Consequently,

$$\begin{aligned} (L_{\text{per}}(f))(x) &= \operatorname{div} \int_{\Omega_{2\rho}} \mathcal{K}_{\text{sm}}(x-y)f(y) \, dy = \operatorname{div} \int_D \mathcal{K}_{\text{sm}}(x-y)f(y) \, dy \\ &= \operatorname{div} \int_D G_{k,\alpha}(x-y)f(y) \, dy = (L_k(f))(x), \quad x \in D. \end{aligned}$$

(b) Assume that $u \in H_\alpha^1(D)$ solves (33) and define $\tilde{u} \in H_{\text{per}}^1(\Omega_R)$ by $\tilde{u} = L_{\text{per}}(q\nabla u + f)$ (where we extended f by zero outside D). Since u solves (33), and due to part (a), we find that $\tilde{u}|_D = u$. Hence $L_{\text{per}}(q\nabla\tilde{u} + f) = L_{\text{per}}(q\nabla u + f)$ in $H_{\text{per}}^1(\Omega_R)$, which yields that

$$\tilde{u} = L_{\text{per}}(q\nabla\tilde{u} + f) \text{ in } H_{\text{per}}^1(\Omega_R). \quad (37)$$

Now, if $f \in L^2(D)^2$ vanishes, then uniqueness of a solution to (33) implies that $u \in H_\alpha^1(D)$ vanishes, too. Obviously, $\tilde{u} = L_{\text{per}}(q\nabla u)$ vanishes, and hence (37) is uniquely solvable. The converse follows directly from (a).

(c) Assume that $u \in H_{\text{per}}^1(\Omega_R)$ solves (36) for $f = q\nabla u^i$. Part (a) implies that the restriction of u to Ω_ρ solves $u - L_k(q\nabla u) = L_k(q\nabla u^i)$ in $H_\alpha^1(\Omega_\rho)$. Hence, Lemma 3.6 implies that u is a weak quasiperiodic solution to $\operatorname{div}((1+q)\nabla u) + k^2 u = -\operatorname{div}(q\nabla u^i)$ in Ω_ρ . Transmission regularity results imply that u belongs to $H_\alpha^2(D) \cap H_\alpha^2(\Omega_\rho \setminus \overline{D})$, and it is well-known that this implies that $u \in H_\alpha^s(\Omega_\rho)$ for $s < 3/2$ (see, e.g., [11, Section 1.2]).

Recall that we assumed that D is compactly contained in Ω_ρ , that is, there is $\varepsilon > 0$ such that $D \subset \Omega_{\rho-2\varepsilon}$. Hence, the representation

$$u(x) = L_{\text{per}}(q\nabla(u + u^i))(x) = \operatorname{div} \int_D \mathcal{K}_{\text{sm}}(x-y)q(y)\nabla(u(y) + u^i(y)) \, dy, \quad x \in \Omega_R \setminus \Omega_{\rho-\varepsilon}$$

shows that the restriction of u to $\Omega_R \setminus \Omega_{\rho-\varepsilon}$ is a smooth quasiperiodic function, since the kernel of the above integral operator is smooth. Consequently, a localization argument shows that $u \in H_{\text{per}}^s(\Omega_R)$ for $s < 3/2$. \square

Next we prove that the operator $I - L_{\text{per}}(q\nabla \cdot)$ from (36) satisfies a Gårding inequality in $H_{\text{per}}^1(\Omega_R)$. For negative material parameters, the result relies on the operator

$$R : H_{\text{per}}^1(\Omega_R) \rightarrow H_{\text{per}}^1(\Omega_R), \quad R(v) = \begin{cases} v - 2E(v) & \text{in } \Omega_R \setminus \overline{D}, \\ -v & \text{in } D, \end{cases} \quad (38)$$

where $E : H_\alpha^1(D) \rightarrow H_\alpha^1(\Omega)$ is the extension operator that we already used in Section 4 (see also Appendix B). Note that Rv indeed belongs to $H_{\text{per}}^1(\Omega_R)$: the jump $[R(v)]_{\partial D}$ vanishes, and $E(v)$ vanishes for $|x_2| > R$.

Theorem 5.3. *Assume that $\sqrt{|q|} \in C^{1,1}(\overline{D})$, that $|q| \geq q_0 > 0$, and that D is of class $C^{2,1}$.*

(a) *If $q > 0$, then there exists $C > 0$ and a compact operator K_+ on $H_{\text{per}}^1(\Omega_R)$ such that*

$$\operatorname{Re} \langle v - L_{\text{per}}(q\nabla v), v \rangle_{H_{\text{per}}^1(\Omega_R)} \geq C \|v\|_{H_{\text{per}}^1(\Omega_R)}^2 - \operatorname{Re} \langle K_+ v, v \rangle_{H_{\text{per}}^1(\Omega_R)} \quad (39)$$

for all $v \in H_{\text{per}}^1(\Omega_R)$.

(b) *If $q < 0$ and if*

$$\frac{\inf_D |q|}{1 + \|E\|_{H_\alpha^1(D) \rightarrow H_\alpha^1(\Omega_R \setminus \overline{D})}^2} > 1 + \|E\|_{H_\alpha^1(D) \rightarrow H_\alpha^1(\Omega_R \setminus \overline{D})}, \quad (40)$$

then there exists $C > 0$ and a compact operator K_- on $H_{\text{per}}^1(\Omega_R)$ such that

$$\operatorname{Re} \langle v - L_{\text{per}}(q\nabla v), R(v) \rangle_{H_{\text{per}}^1(\Omega_R)} \geq C \|v\|_{H_{\text{per}}^1(\Omega_R)}^2 - \operatorname{Re} \langle K_- v, v \rangle_{H_{\text{per}}^1(\Omega_R)} \quad (41)$$

for all $v \in H_{\text{per}}^1(\Omega_R)$.

Remark 5.4. *The idea of the proof is to split the integrals defining the inner product on the left of (39) into the three integrals on D , $\Omega_\rho \setminus \overline{D}$, and on $\Omega_R \setminus \overline{\Omega_\rho}$. For the term on D one exploits the Gårding inequalities from Theorem 4.8. The terms on $\Omega_\rho \setminus \overline{D}$ and on $\Omega_R \setminus \overline{\Omega_\rho}$ can be shown to be compact and positive up to compact perturbations, respectively.*

Proof. (a) Let $v \in H_{\text{per}}^1(\Omega_R)$. First, we split up the integrals arising from the inner product on the left of (39) into integrals on D , on $\Omega_\rho \setminus \overline{D}$, and on $\Omega_R \setminus \overline{\Omega_\rho}$. Second, we use the Gårding inequality from Theorem 4.8 to find that

$$\begin{aligned} \operatorname{Re} \langle v - L_{\text{per}}(q\nabla v), v \rangle_{H_{\text{per}}^1(\Omega_R)} &\geq C \|v\|_{H_\alpha^1(D)}^2 + \langle K v, v \rangle_{H_\alpha^1(D)} + \|v\|_{H_\alpha^1(\Omega_R \setminus \overline{D})}^2 \\ &\quad - \operatorname{Re} [\langle L_{\text{per}}(q\nabla v), v \rangle_{H_\alpha^1(\Omega_R \setminus \overline{\Omega_\rho})} + \langle L_{\text{per}}(q\nabla v), v \rangle_{H_\alpha^1(\Omega_\rho \setminus \overline{D})}]. \end{aligned} \quad (42)$$

Recall that the operator K is compact on $H_\alpha^1(D)$. Further, the evaluation of $L_{\text{per}}(q\nabla \cdot)$ on $\Omega_R \setminus \overline{\Omega_\rho}$ defines a compact integral operator mapping $H_\alpha^1(D)$ to $H_\alpha^1(\Omega_R \setminus \overline{\Omega_\rho})$, because the (periodic) kernel of this integral operator is smooth. (This argument requires the smooth kernel \mathcal{K}_{sm} introduced in the beginning of this section.) Unfortunately, the last term in (42) cannot be written as a compact sesquilinear form, and needs a detailed investigation.

For $x \in \Omega_\rho \setminus \overline{D}$ and $y \in D$ the kernel $\mathcal{K}_{\text{sm}}(x-y)$ equals $G_{k,\alpha}(x-y)$, which is a smooth function of $x \in \Omega_\rho \setminus \overline{D}$ and $y \in D$. Moreover, $\Delta G_{k,\alpha}(x-y) + k^2 G_{k,\alpha}(x-y) = 0$ for $x \neq y$. Integration by parts in $\Omega_\rho \setminus \overline{D}$ shows that

$$\begin{aligned} L_k(q\nabla v)(x) &= \operatorname{div} \int_D G_{k,\alpha}(x-y) q(y) \nabla v(y) \, dy \\ &= - \int_D \nabla_y G_{k,\alpha}(x-y) \cdot \nabla(qv)(y) \, dy + \int_D \nabla_y G_{k,\alpha}(x-y) \cdot \nabla q(y) v(y) \, dy \\ &= -k^2 \int_D G_{k,\alpha}(x-y) q(y) v(y) \, dy - L_k(v\nabla q)(x) \\ &\quad - \int_{\partial D} \frac{\partial G_{k,\alpha}(x-y)}{\partial \nu(y)} \gamma_{\text{int}}(q)(y) \gamma(v)(y) \, ds, \quad x \in \Omega_\rho \setminus \overline{D}, \end{aligned}$$

where ν is as usual the exterior normal vector to D . The integral operator appearing in the last term of the last equation is the double layer potential DL, defined by

$$\operatorname{DL}(\psi) = \int_{\partial D} \frac{\partial G_{k,\alpha}(\cdot - y)}{\partial \nu(y)} \psi(y) \, ds, \quad \text{in } \Omega \setminus \partial D.$$

It is well-known that DL defines a bounded operator from $H_\alpha^{1/2}(\partial D)$ into $H_\alpha^1(\Omega_R \setminus \overline{D})$ and into $H_\alpha^1(D)$ (see, e.g., [1, 31]). This implies that the jump of the double-layer potential

$$T\psi := [\operatorname{DL}\psi]_{\partial D} = \gamma_{\text{ext}}(\operatorname{DL}\psi) - \gamma_{\text{int}}(\operatorname{DL}\psi)$$

from the outside of D to the inside of D is a bounded operator on $H_\alpha^{1/2}(\partial D)$. It is well-known that in our case T is even a compact operator on $H^{1/2}(\partial D)$, since D is of class $C^{2,1}$. Additionally, the equality $\gamma_{\text{ext}}(\operatorname{DL}\psi) = -\psi/2 + T\psi$ holds for $\psi \in H_\alpha^{1/2}(\partial D)$.

We will from now on skip the trace operators to ease notation, e.g., we write $\text{DL}(qv)$ instead of $\text{DL}(\gamma_{\text{int}}(q)\gamma(v))$. Then

$$-\langle \nabla L_k(q\nabla v), \nabla v \rangle_{L^2(\Omega_\rho \setminus \overline{D})} = \langle k^2 \nabla V_k(qv) + \nabla L_k(v\nabla q), \nabla v \rangle_{L^2(\Omega_\rho \setminus \overline{D})} + \langle \nabla \text{DL}(qv), \nabla v \rangle_{L^2(\Omega_\rho \setminus \overline{D})}, \quad \text{for } v \in H_{\text{per}}^1(\Omega_R). \quad (43)$$

The mapping properties of V_k shown in Lemma 3.5 and the smoothness of q imply that $v \mapsto k^2 \nabla V_k(v) + \nabla L_k(v\nabla q)$ is compact from $H_{\text{per}}^1(\Omega_R)$ into $L^2(D)$. To finish the proof of part (a) we show that the last term in (43) can be written as a sum of a positive and compact term. For simplicity, we set $w = \text{DL}(qv)$. Then

$$\begin{aligned} \langle \nabla \text{DL}(qv), \nabla v \rangle_{L^2(\Omega_\rho \setminus \overline{D})} &= \int_{\Omega_\rho \setminus \overline{D}} \nabla w \cdot \nabla \overline{v} \, dx \\ &= k^2 \int_{\Omega_\rho \setminus \overline{D}} w \overline{v} \, dx - \int_{\partial D} \frac{\partial w}{\partial \nu} \overline{v} \, ds + \int_{\Gamma_\rho} \frac{\partial w}{\partial x_2} \overline{v} \, ds - \int_{\Gamma_{-\rho}} \frac{\partial w}{\partial x_2} \overline{v} \, ds. \end{aligned} \quad (44)$$

The above jump relation shows that

$$\begin{aligned} - \int_{\partial D} \frac{\partial w}{\partial \nu} \overline{v} \, ds &= 2 \int_{\partial D} \frac{\partial w \overline{w}}{\partial \nu q} \, ds - 2 \int_{\partial D} \frac{\partial w \overline{T(qv|_{\partial D})}}{\partial \nu q} \, ds \\ &= 2 \int_D \nabla w \cdot \nabla \frac{\overline{w}}{q} \, dx + 2 \int_D \Delta w \frac{\overline{w}}{q} \, dx - 2 \int_{\partial D} \frac{\partial w \overline{T(qv)}}{\partial \nu q} \, ds \\ &= 2 \int_D \frac{|\nabla w|^2}{q} \, dx + 2 \int_D (\nabla q^{-1} \cdot \nabla w - k^2 \frac{w}{q}) \overline{w} \, dx - 2 \int_{\partial D} \frac{\partial w \overline{T(qv)}}{\partial \nu q} \, ds. \end{aligned}$$

Combining the last computation with (44) shows that

$$\begin{aligned} \langle \nabla \text{DL}(qv|_{\partial D}), \nabla v|_{\Omega_\rho \setminus \overline{D}} \rangle_{L^2(\Omega_\rho \setminus \overline{D})} &= 2 \int_D \frac{|\nabla w|^2}{q} \, dx + k^2 \int_{\Omega_\rho \setminus \overline{D}} w \overline{v} \, dx \\ &\quad + 2 \int_D \left(\nabla q \cdot \nabla w - k^2 \frac{w}{q} \right) \overline{w} \, dx - 2 \int_{\partial D} \frac{\partial w \overline{T(qv)}}{\partial \nu q} \, ds + \left(\int_{\Gamma_\rho} - \int_{\Gamma_{-\rho}} \right) \frac{\partial w}{\partial x_2} \overline{v} \, ds. \end{aligned} \quad (45)$$

Using Lemma 4.3, the terms in the second and third line of the last equation can be rewritten as $\langle K_1 v, v \rangle_{H_{\text{per}}^1(\Omega_R)}$ where K_1 is a compact operator on $H_{\text{per}}^1(\Omega_R)$. The mapping $v \mapsto \int_D |\nabla w|^2/q \, dx$ is obviously positive if $q > 0$. In consequence, (42) and (43) show that (39) holds.

(b) Recall that $R(v) = v - 2E(v)$ in $\Omega_R \setminus \overline{D}$ and set

$$\lambda_2 := \|E\|_{H_\alpha^1(D) \rightarrow H_\alpha^1(\Omega_R \setminus \overline{D})}.$$

Exactly as in the first part of the proof we split

$$\langle v - L_{\text{per}}(q\nabla v), R(v) \rangle = \langle v - L_{\text{per}}(q\nabla v), R(v) \rangle_{H_\alpha^1(\Omega_R \setminus \overline{D})} - \langle v - L_k(q\nabla v), v \rangle_{H_\alpha^1(D)}$$

and estimate that

$$\begin{aligned}
\operatorname{Re} \langle v - L_{\text{per}}(q\nabla v), R(v) \rangle &\geq C \|v\|_{H_\alpha^1(D)}^2 + \langle K_- v, v \rangle_{H_\alpha^1(D)} + \|v\|_{H_\alpha^1(\Omega_R \setminus \overline{D})}^2 \\
&\quad - 2\operatorname{Re} \langle v, E(v) \rangle_{H_\alpha^1(\Omega_R \setminus \overline{D})} - \operatorname{Re} \langle L_{\text{per}}(q\nabla v), R(v) \rangle_{H_\alpha^1(\Omega_R \setminus \overline{\Omega}_\rho)} \\
&\quad - \operatorname{Re} \langle L_{\text{per}}(q\nabla v), R(v) \rangle_{H_\alpha^1(\Omega_\rho \setminus \overline{D})} \\
&\geq (C - \beta^{-1}\lambda_2) \|v\|_{H_\alpha^1(D)}^2 + (1 - \beta) \|v\|_{H_\alpha^1(\Omega_R \setminus \overline{D})}^2 + \langle K_- v, v \rangle_{H_\alpha^1(D)} \\
&\quad - \operatorname{Re} \langle L_{\text{per}}(q\nabla v), R(v) \rangle_{H_\alpha^1(\Omega_R \setminus \overline{\Omega}_\rho)} \\
&\quad - \operatorname{Re} \langle L_k(q\nabla v), R(v) \rangle_{H_\alpha^1(\Omega_\rho \setminus \overline{D})}
\end{aligned}$$

where $\beta \in (0, 1)$ and K_- is a compact operator on $H_\alpha^1(D)$. The constant C is the same as the one appearing in Theorem 4.8(b), that is,

$$C - \beta^{-1}\lambda_2 = \frac{(1 - \varepsilon) \inf_D |q|}{1 + \|E\|_{H_\alpha^1(D) \rightarrow H_\alpha^1(\Omega_R \setminus \overline{D})}^2} - 1 - \beta^{-1} \|E\|_{H_\alpha^1(D) \rightarrow H_\alpha^1(\Omega_R \setminus \overline{D})}, \quad \varepsilon > 0, \beta \in (0, 1).$$

Obviously, if condition (40) holds, then one can choose $\varepsilon > 0$ small enough and $\beta \in (0, 1)$ close enough to one such that $C - \beta^{-1}\lambda_2 > 0$.

In part (a) we have already seen that $L_{\text{per}}(q\nabla v)$ is compact from $H_{\text{per}}^1(\Omega_R)$ into $H_\alpha^1(\Omega_R \setminus \overline{\Omega}_\rho)$. To conclude the proof we need again to investigate

$$\begin{aligned}
-\langle \nabla L_k(q\nabla v), \nabla R(v) \rangle_{L^2(\Omega_\rho \setminus \overline{D})} &= \langle k^2 \nabla V_k(qv) + \nabla L_k(v\nabla q), \nabla R(v) \rangle_{L^2(\Omega_\rho \setminus \overline{D})} \\
&\quad + \langle \nabla \text{DL}(qv|_{\partial D}), \nabla R(v) \rangle_{L^2(\Omega_\rho \setminus \overline{D})}. \quad (46)
\end{aligned}$$

Again, we already know from part (a) that $v \mapsto k^2 \nabla V_k(qv) + \nabla L_k(v\nabla q)$ is compact from $H_{\text{per}}^1(\Omega_R)$ into $L^2(\Omega_\rho \setminus \overline{D})$. The third term in (46) is again treated using an integration by parts showing that this term is positive up to compact perturbations. If we set $w = \text{DL}(qv)$, then

$$\begin{aligned}
\langle \nabla \text{DL}(qv|_{\partial D}), \nabla R(v) \rangle_{L^2(\Omega_\rho \setminus \overline{D})} &= \int_{\Omega_\rho \setminus \overline{D}} \nabla w \cdot \nabla \overline{R(v)} \, dx \\
&= k^2 \int_{\Omega_\rho \setminus \overline{D}} w \overline{R(v)} \, dx - \int_{\partial D} \frac{\partial w}{\partial \nu} \overline{R(v)} \, ds + \int_{\Gamma_\rho} \frac{\partial w}{\partial x_2} \overline{R(v)} \, ds - \int_{\Gamma_{-\rho}} \frac{\partial w}{\partial x_2} \overline{R(v)} \, ds.
\end{aligned}$$

By construction, $\gamma(R(v)) = \gamma(v - 2E(v)) = -\gamma(v)$. Hence, a computation analogous to (45) shows that

$$\begin{aligned}
-\int_{\partial D} \frac{\partial w}{\partial \nu} \overline{R(v)} \, ds &= \int_{\partial D} \frac{\partial w}{\partial \nu} \overline{v} \, ds = 2 \int_D \frac{|\nabla w|^2}{|q|} \, dx \\
&\quad - 2 \int_D (\nabla q^{-1} \cdot \nabla \overline{w} - k^2 \frac{\overline{w}}{q}) w \, dx - 2 \int_{\partial D} \frac{\partial w}{\partial \nu} \frac{\overline{T(qv)}}{q} \, ds \quad (47)
\end{aligned}$$

where we exploited the assumption that q is negative. \square

6 Discretization of the Periodic Integral Equation

In this section we consider the discretization of the periodized integral equation (36) in spaces of trigonometric polynomials. Convergence theory for this discretization is a consequence of the

Gårding inequalities shown in Theorem 5.3. The spectral scheme we use is similar to the collocation scheme from [33]. However, for our purpose we use a Galerkin variant similar to the one from [18]. The usual convergence theory for the collocation methods does not apply here due to the discontinuous material parameter.

For $N \in \mathbb{N}$ we define $\mathbb{Z}_N^2 = \{j \in \mathbb{Z}^2 : -N/2 < j_{1,2} \leq N/2\}$ and

$$\mathcal{T}_N = \text{span}\{\varphi_j : j \in \mathbb{Z}_N^2\},$$

where $\varphi_j \in L^2(\Omega_R)$ are the α -quasi-periodic basis functions from (35). Since $\{\varphi_j\}_{j \in \mathbb{N}}$ is an orthogonal basis of $H_{\text{per}}^1(\Omega_R)$, the union $\cup_{N \in \mathbb{N}} \mathcal{T}_N$ is dense in $H_{\text{per}}^1(\Omega_R)$. We also consider the orthogonal projection P_N from $H_{\text{per}}^1(\Omega_R)$ onto \mathcal{T}_N ,

$$P_N(v) = \sum_{j \in \mathbb{Z}_N^2} \hat{v}(j) \varphi_j,$$

where $\hat{v}(j)$ denotes as above the j th Fourier coefficient. The next proposition recalls the standard convergence result for Galerkin discretizations of equations that satisfy a Gårding inequality, see, e.g. [30, Theorem 4.2.9], combined with the regularity result from Theorem 5.2(c).

Proposition 6.1. *Assume that q satisfies the assumptions of Theorem 5.3 (a) or (b) and that (21) is uniquely solvable. Denote the unique solution in $H_{\text{per}}^1(\Omega_R)$ to (36) by u . Then there is $N_0 \in \mathbb{N}$ such that the finite-dimensional problem to find $u_N \in \mathcal{T}_N$ such that*

$$(a) \quad \langle u_N - L_{\text{per}}(q\nabla u_N), w_N \rangle_{H_{\text{per}}^1(\Omega_R)} = \langle f, w_N \rangle_{H_{\text{per}}^1(\Omega_R)} \quad \text{for all } w_N \in \mathcal{T}_N, \quad \text{or} \quad (48)$$

$$(b) \quad \langle u_N - L_{\text{per}}(q\nabla u_N), R(w_N) \rangle_{H_{\text{per}}^1(\Omega_R)} = \langle f, R(w_N) \rangle_{H_{\text{per}}^1(\Omega_R)} \quad \text{for all } w_N \in \mathcal{T}_N, \quad (49)$$

possesses a unique solution for all $N \geq N_0$ and $f \in H_{\text{per}}^1(\Omega_R)$. Additionally, in both cases

$$\|u_N - u\|_{H_{\text{per}}^1(\Omega_R)} \leq C \inf_{w_N \in \mathcal{T}_N} \|w_N - u\|_{H_{\text{per}}^1(\Omega_R)} \leq CN^{-s} \|u\|_{H_{\text{per}}^{1+s}(\Omega_R)}, \quad 0 \leq s < 1/2,$$

with a constant C independent of $N \geq N_0$.

Remark 6.2. *The convergence rate increases to $s + 1 - t$ if one measures the error in the weaker Sobolev norms of $H_{\text{per}}^t(\Omega_R)$, $1/2 < t < 1$. This can be shown using adjoint estimates (see, e.g. [30, Section 4.2] for the general technique). The (linear) rate saturates at $t = 1/2$, since the integral operator is not bounded on $H_{\text{per}}^t(\Omega_R)$ for $t < 1/2$. Hence, the L^2 -error generally converges to zero at a linear rate.*

If the contrast q is negative, the discretization (49) involves the isomorphism R . Interestingly, this is not necessary for convergence of the scheme, at least not for the right hand sides $f = L_{\text{per}}(q\nabla u^i)$ that are of physical interest.

Proposition 6.3. *Assume that q satisfies the assumptions of Theorem 5.3 (a) or (b) and that (21) is uniquely solvable. For an arbitrary right-hand side of the form $f = L_{\text{per}}(q\nabla u^i)$, where u^i is a smooth quasi-periodic incident field, we denote the unique solution in $H_{\text{per}}^1(\Omega_R)$ to (36) by u . Then there is $N_0 \in \mathbb{N}$ independent of u^i such that the finite-dimensional problem to find $u_N \in \mathcal{T}_N$ solving*

$$\langle u_N - L_{\text{per}}(q\nabla u_N), w_N \rangle_{H_{\text{per}}^1(\Omega_R)} = \langle f, w_N \rangle_{H_{\text{per}}^1(\Omega_R)} \quad \text{for all } w_N \in \mathcal{T}_N \quad (50)$$

possesses a unique solution $u_N \in \mathcal{T}_N$, and $\|u_N - u\|_{H_{\text{per}}^1(\Omega_R)} \leq CN^{-s} \|f\|_{H_{\text{per}}^{1+s}(\Omega_R)}$, $0 \leq s < 1/2$.

Proof. In this proof, $\|\cdot\|$ denotes either the norm or the operator norm on $H_{\text{per}}^1(\Omega_R)$ and $\langle \cdot, \cdot \rangle$ is the corresponding inner product.

It is obvious that the Gårding inequality (41) implies a Gårding inequality for the corresponding transposed sesquilinear form. Further, the unique solvability of the Lippmann-Schwinger integral equation (21) implies by Theorem 5.2(b) $I - L_{\text{per}}(q\nabla \cdot)$ is an isomorphism on $H_{\text{per}}^1(\Omega_R)$; by construction, R is an isomorphism, too. Standard Galerkin convergence theory [30] implies that there is $N_0 \in \mathbb{N}$ such that for $N \geq N_0$ and any $w_N \in \mathcal{T}_N$ there is a unique solution $z_N \in \mathcal{T}_N$ to

$$\langle u_N - L_{\text{per}}(q\nabla u_N), R(z_N) \rangle = \langle u_N - L_{\text{per}}(q\nabla u_N), w_N \rangle \quad \text{for all } u_N \in \mathcal{T}_N. \quad (51)$$

The mapping $S_N : w_N \mapsto z_N$ is hence a well-defined linear operator on \mathcal{T}_N . The operator norms $\|S_N\|$ are uniformly bounded in N , because the norm of the solution operator to (51) is uniformly bounded in N .

The mapping S_N is injective: If $z_N = S_N(w_N) = 0$, then $\langle u_N - L_{\text{per}}(q\nabla u_N), R(z_N) \rangle = 0$ for all $u_N \in \mathcal{T}_N$. Obviously, one solution to this equation is the trivial solution; uniqueness of solution to (51) implies that $w_N = 0$. Since $w_N \mapsto S_N(w_N)$ is injective on the finite-dimensional space \mathcal{T}_N , this mapping is onto. We denote its inverse by S_N^{-1} .

Replacing w_N by $S_N^{-1}z_N$ in (51) shows that

$$\langle u_N - L_{\text{per}}(q\nabla u_N), R(z_N) \rangle = \langle u_N - L_{\text{per}}(q\nabla u_N), S_N^{-1}z_N \rangle \quad \text{for all } u_N, z_N \in \mathcal{T}_N.$$

In consequence,

$$\langle u_N - L_{\text{per}}(q\nabla u_N), R(z_N) \rangle = \langle (S_N^{-1})^* P_N [u_N - L_{\text{per}}(q\nabla u_N)], z_N \rangle \quad \text{for all } u_N, z_N \in \mathcal{T}_N.$$

Firstly choosing $z_N = (S_N^{-1})^* P_N [u_N - L_{\text{per}}(q\nabla u_N)]$, and secondly applying the Cauchy-Schwarz inequality yields the bound

$$\| (S_N^{-1})^* P_N [u_N - L_{\text{per}}(q\nabla u_N)] \| \leq \|R\| \|I - L_{\text{per}}(q\nabla \cdot)\| \|u_N\|. \quad (52)$$

Hence, the operator norms of $u_N \mapsto (S_N^{-1})^* P_N [u_N - L_{\text{per}}(q\nabla u_N)]$ are uniformly bounded in $N \geq N_0$.

Since S_N^{-1} exists on \mathcal{T}_N , solving (49) is equivalent to solving

$$\langle v_N - L_{\text{per}}(q\nabla v_N), R(S_N w_N) \rangle = \langle f, R(S_N w_N) \rangle \quad \text{for all } w_N \in \mathcal{T}_N,$$

that is, by the definition of S_N via (51),

$$\langle v_N - L_{\text{per}}(q\nabla v_N), w_N \rangle = \langle S_N^* P_N R^* f, w_N \rangle \quad \text{for all } w_N \in \mathcal{T}_N. \quad (53)$$

R^* and S_N^* are isomorphisms on $H_{\text{per}}^1(\Omega_R)$ and on \mathcal{T}_N , respectively, that is, the operator $S_N^* P_N R^*$ is onto from $H_{\text{per}}^1(\Omega_R)$ into \mathcal{T}_N . Hence, for $N \geq N_0$ and all $f \in H_{\text{per}}^1(\Omega)$, there is $u_N \in \mathcal{T}_N$ such that

$$\langle u_N - L_{\text{per}}(q\nabla u_N), w_N \rangle = \langle f, w_N \rangle \quad \text{for all } w_N \in \mathcal{T}_N. \quad (54)$$

Recall that the solution v_N to (53) (or, equivalently, to (49)) is uniformly bounded by $\|v_N\| \leq C\|f\|$. The solution u_N to (54) satisfies (53) with f replaced by $R^*(S_N^*)^{-1}P_N f$. (Recall that $R^2 = I$, that is $R^* = (R^*)^{-1}$.) In particular, (53) implies that

$$\|u_N\| \leq C\|R^*(S_N^*)^{-1}P_N f\|. \quad (55)$$

To estimate the error $u_N - u$ for the special right-hand side $f = L_{\text{per}}(q\nabla u^i)$, we estimate $d_N := u_N - v_N$ (since we already have an error estimate for $\|v_N - u\|$ due to Theorem 6.1). Let us

first note that for $f = L_{\text{per}}(q\nabla u^i)$ there exists $g \in H_{\text{per}}^1(\Omega_R)$ such that $g - L_{\text{per}}(q\nabla g) = L_{\text{per}}(q\nabla u^i)$. Due to Theorem 5.2(c), g belongs to $H_{\text{per}}^{1+s}(\Omega_R)$ for all $s < 1/2$. Then

$$\begin{aligned} \langle d_N - L_{\text{per}}(q\nabla d_N), w_N \rangle &= \langle f, w_N \rangle_{H_{\text{per}}^1(\Omega_R)} - \langle f, RS_N w_N \rangle \\ &= \langle g - L_{\text{per}}(q\nabla g), w_N - RS_N w_N \rangle \\ &\stackrel{(*)}{=} \langle (I - L_{\text{per}}(q\nabla \cdot))(g - P_N g), (I - RS_N)w_N \rangle \\ &= \langle (I - RS_N)^*(I - L_{\text{per}}(q\nabla \cdot))(g - P_N g), w_N \rangle \quad \text{for all } w_N \in \mathcal{T}_N, \end{aligned}$$

where we used the Galerkin orthogonality from (51) (with $u_N = P_N g$) in (*). Hence, d_N solves problem (54) with right-hand side $f = (I - RS_N)^*(I - L_{\text{per}}(q\nabla \cdot))(g - P_N g)$ and (55) yields the estimate

$$\begin{aligned} \|d_N\| &= \|v_N - u_N\| \leq C \|R^*(S_N^*)^{-1} P_N (I - RS_N)^*(I - L_{\text{per}}(q\nabla \cdot))(g - P_N g)\| \\ &\leq \|R^*\| \| (S_N^*)^{-1} P_N (I - L_{\text{per}}(q\nabla \cdot))(g - P_N g) \| + \| (I - L_{\text{per}}(q\nabla \cdot))(g - P_N g) \|. \end{aligned}$$

Recall from (52) that the operator norms $\| (S_N^*)^{-1} P_N (I - L_{\text{per}}(q\nabla \cdot)) \|$ are uniformly bounded by $\|R\| \|I - L_{\text{per}}(q\nabla \cdot)\|$. Hence

$$\|d_N\| \leq C \|g - P_N g\| \leq CN^{-s} \|g\|_{H_{\text{per}}^{1+s}(\Omega_R)} \leq CN^{-s} \|f\|_{H_{\text{per}}^{1+s}(\Omega_R)}.$$

□

7 Fully Discrete Formulas and Numerical Experiments

In this section we present the fully discrete versions of the Galerkin discretization of the Lippmann-Schwinger integral equation and show some numerical examples.

Applying P_N to the infinite-dimensional problem (36) we obtain the discrete problem to find $u_N \in \mathcal{T}_N$ such that

$$u_N - L_{\text{per}}(P_N(q\nabla u_N)) = L_{\text{per}}(P_N f), \quad (56)$$

where we already exploited that P_N commutes with the convolution-like operator L_{per} .

Fast methods to evaluate the discretized operator in (56) exploit that the application of L_{per} to a trigonometric polynomial in \mathcal{T}_N can be computed explicitly using a (α -quasi-periodic) discrete Fourier transform \mathcal{F}_N . This transform maps point values of a trigonometric polynomial to the Fourier coefficients of the polynomial. If we denote by $a \bullet b$ the componentwise multiplication of two matrices, and if $h := (2\pi/N, 4\pi R/N)^\top$, then

$$\hat{v}_N(j) = \frac{\sqrt{4\pi R}}{N^2} \sum_{l \in \mathbb{Z}_N^2} v_N(l \bullet h) \exp(-2\pi i (j_1 + \alpha, j_2)^\top \cdot l/N), \quad j \in \mathbb{Z}_N^2.$$

This defines the transform \mathcal{F}_N mapping $(v_N(j \bullet h))_{j \in \mathbb{Z}_N^2}$ to $(\hat{v}_N(j))_{j \in \mathbb{Z}_N^2}$. The inverse \mathcal{F}_N^{-1} is explicitly given by

$$v_N(j \bullet h) = \frac{1}{\sqrt{4\pi R}} \sum_{l \in \mathbb{Z}_N^2} \hat{v}_N(l) \exp(2\pi i (l_1 + \alpha, l_2)^\top \cdot j/N), \quad j \in \mathbb{Z}_N^2.$$

Both \mathcal{F}_N and its inverse are linear operators on $\mathbb{C}_N^2 = \{(c_n)_{n \in \mathbb{Z}_N^2} : c_n \in \mathbb{C}\}$. The restriction operator $R_{N,M}$ from \mathbb{C}_N^2 to \mathbb{C}_M^2 , $N > M$, is defined by

$$R_{N,M}(a) = b, \quad b(j) = a(j) \text{ for } j \in \mathbb{Z}_M^2.$$

The extension operator $E_{M,N}$ from \mathbb{C}_M^2 to \mathbb{C}_N^2 , $M < N$, is

$$E_{M,N}(a) = b, \quad b(j) = a(j) \text{ for } j \in \mathbb{Z}_M^2 \text{ and } b(j) = 0 \text{ else.}$$

Lemma 7.1. *The Fourier coefficients of $q\partial_\ell u_N$, $\ell = 1, 2$, are given by*

$$(\widehat{q\partial_\ell u_N}(j))_{j \in \mathbb{Z}_N^2} = R_{3N,N} \mathcal{F}_{3N} [\mathcal{F}_{3N}^{-1}(E_{2N,3N}(\hat{q}_{2N}(j))_{j \in \mathbb{Z}_N^2}) \bullet \mathcal{F}_{3N}^{-1}(E_{N,3N}(w_\ell(j)\hat{u}_N(j))_{j \in \mathbb{Z}_N^2})]$$

where $w_1(j) = i(j_1 + \alpha)$ and $w_2(j) = ij_2\pi/R$ for $j \in \mathbb{Z}^2$.

Proof. For $u_N \in \mathcal{T}_N$, $j \in \mathbb{Z}^2$, and $\ell = 1, 2$, we compute that

$$\begin{aligned} \widehat{q\partial_\ell u_N}(j) &= \int_{\Omega_R} q\partial_\ell u_N \overline{\varphi_j} dx = \sum_{m \in \mathbb{Z}_N^2} \widehat{\partial_\ell u_N}(m) \int_{\Omega_R} q \overline{\varphi_j} \varphi_m dx \\ &= (4\pi R)^{-1} \sum_{m \in \mathbb{Z}_N^2} \widehat{\partial_\ell u_N}(m) \int_{\Omega_R} q(x) e^{-i[(j_1-m_1)x_1 + (j_2-m_2)x_2\pi/R]} dx \\ &= (4\pi R)^{-1/2} \sum_{m \in \mathbb{Z}_N^2} \widehat{\partial_\ell u_N}(m) \hat{q}(j-m). \end{aligned} \quad (57)$$

If $j \in \mathbb{Z}_N^2$, then the coefficient $\widehat{q\partial_\ell u_N}(j)$ merely depends on $\hat{q}(m)$ for $m \in \mathbb{Z}_{2N}^2$. Hence, $\widehat{q\partial_\ell u_N}(j) = q_{2N} \widehat{\partial_\ell u_N}(j)$ for $j \in \mathbb{Z}_N^2$. Obviously, $q_{2N} \partial_\ell u_N$ belongs to \mathcal{T}_{3N} . Hence, the Fourier coefficients of $q_{2N} \partial_\ell u_N$ are given by \mathcal{F}_{3N} applied to the grid values of this function at $j \bullet h$, $j \in \mathbb{Z}_{3N}^2$. The grid values of $\widehat{\partial_\ell u_N}$ are given by $\mathcal{F}_{3N}^{-1}(E_{N,3N}(\widehat{\partial_\ell u_N}(j))_{j \in \mathbb{Z}_N^2})$, and the grid values of q_{2N} can be computed analogously. Finally, taking a partial derivative with respect to x_1 or x_2 of u yields a multiplication of the j th Fourier coefficient $\hat{u}(j)$ by $i(j_1 + \alpha)$ and $ij_2\pi/R$, respectively. \square

In Lemma 3.2 we computed the Fourier coefficients of the kernel \mathcal{K}_R . The kernel \mathcal{K}_{sm} used to define the periodized potential L_{per} is the product of \mathcal{K}_R with the smooth function χ (see (34)). Hence, the Fourier coefficients of \mathcal{K}_{sm} is a convolution of the $\hat{\mathcal{K}}_R(j)$ with $\hat{\chi}(j_2) = (4\pi R)^{-1/2} \int_{-R}^R \exp(-ij_2\pi x_2/R) \chi(x_2) dx_2$,

$$\hat{\mathcal{K}}_{\text{sm}}(j) = \frac{1}{(4\pi R)^{1/2}} \sum_{m \in \mathbb{Z}_N^2} \hat{\mathcal{K}}_R(j_1, m_2) \hat{\chi}(j_2 - m_2), \quad j \in \mathbb{Z}^2.$$

The latter formula can be seen by a computation similar to (57). Note that χ is a smooth function, which means that the Fourier coefficients $\hat{\chi}$ in the last formula are rapidly decreasing, that is, the truncation the last series converges rapidly to the exact value. The convolution structure of L_{per} finally shows that

$$(\widehat{L_{\text{per}}f})(j) = (4\pi R)^{1/2} \hat{\mathcal{K}}_{\text{sm}}(j) \left[i(j_1 + \alpha) \hat{f}_1(j) + \frac{ij_2\pi}{R} \hat{f}_2(j) \right] \quad \text{for } f = (f_1, f_2)^\top \in L^2(\Omega_R)^2. \quad (58)$$

The finite-dimensional operator $u_N \mapsto L_{\text{per}}(P_N(q\nabla u_N))$ can now be evaluated by combining the formula of Lemma (7.1) with (58). The linear system (56) can then be solved using iterative methods (as GMRES, for instance). Whenever one uses iterative techniques, one would of course like to precondition the linear system. The usual multi-grid preconditioning technique for integral equations of the second kind (see, e.g., [12] or [29]) does not apply here, since the integral operator is not compact. For the numerical experiments presented below, we simply used an unpreconditioned

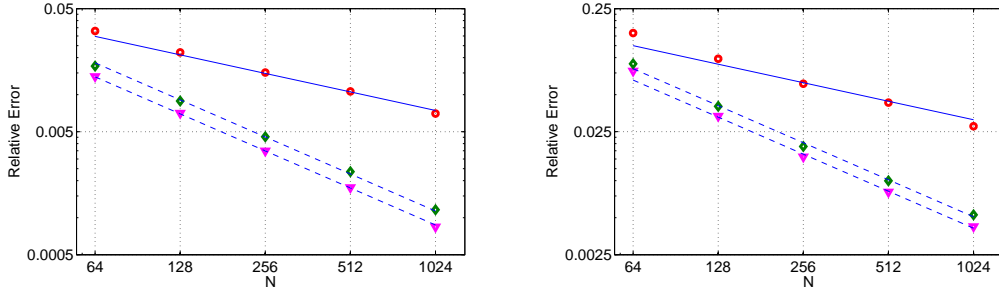


Figure 4: Relative error of the approximated solution and the reference solution measured in H_{per}^s -norm for scattering from a strip. Circles, kites, triangles correspond to $s = 1$, $s = 0.5$ and $s = 0$, respectively. The continuous line and the dotted lines indicate the convergence order 0.5 and 1, respectively. (a) The contrast q equals 2: relative error versus $N = 2^n$, $n = 6, \dots, 10$. (b) The contrast q equals $-2.5 + 5i$: relative error versus $N = 2^n$, $n = 6, \dots, 10$.

GMRES algorithm. All the computations in the two following experiments were done on a machine with an Intel Core 2 Quad 2.66 GHz processor and 8 GB memory using MATLAB.

In the first numerical experiment we confirm the theoretical convergence statements from Propositions 6.1 and 6.3. Recall that we aim to compute the scattered field for an incident field $u^i(x_1, x_2) = \exp(ik(\cos(\theta)x_1 - \sin(\theta)x_2))$ with incident angle θ , where we choose here $k = \pi/2$ and $\theta = \pi/2$. We approximate the solution in \mathcal{T}_N where $N = 2^n$ for $n = 6, \dots, 10$. For this example, $D = (-\pi, \pi) \times (-1, 1)$ is a strip and we choose $\Omega_R = (-\pi, \pi) \times (-3, 3)$. We consider two cases: (a) the contrast q is equal to 2 in D and (b) the contrast q is equal to $-2.5 + 5i$ in D . For this setting one can explicitly compute the scattered field. The restarted GMRES iteration (the restart parameter equals 20) is stopped when the relative residual is less than 10^{-5} . In the Figure 4 we show the relative error between the numerical and the analytical solution in the norms $H_{\text{per}}^s(\Omega_R)$ where $s = 0, 0.5, 1$. The relative error measured in the norm $H_{\text{per}}^1(\Omega_R)$ fits quite well to the theoretical statement in Proposition 6.1. Furthermore, if one measures the relative error in the norm $H_{\text{per}}^s(\Omega_R)$ for $s = 0$ and $s = 0.5$ the experiment confirms the statement of Remark 6.2. To give an impression about computation times, the results in Figure 4(a) took about 0.5, 3.6, 7.5, 29.6 and 105.2 seconds for $N = 2^n$, $n = 6, \dots, 10$.

In the second numerical experiment, we consider a more complicated periodic structure, where kite-shaped inclusions are periodically aligned. The boundary of the inclusion is parametrized by $(z_1(t), z_2(t)) = (1.5 \cos(t) + \cos(2t) - 0.65, \sin(t))$ where $t \in [0, 2\pi]$. Assume that the contrast q equals a constant, say q_0 , inside the structure. Its Fourier coefficients can be approximated using Green's formula as follows,

$$\begin{aligned} \hat{q}(j) &= \frac{1}{\sqrt{4\pi R}} \int_{\Omega_R} q(x) e^{-ij_1 x_1 - i\frac{j_2 \pi}{R} x_2} dx = \frac{q_0}{\sqrt{4\pi R}} \int_D e^{-ij_1 x_1 - i\frac{j_2 \pi}{R} x_2} dx \\ &= \frac{iRq_0}{j_2 \pi \sqrt{4\pi R}} \int_{\partial D} \nu_2(x) e^{-ij_1 x_1 - i\frac{j_2 \pi}{R} x_2} ds \\ &= \frac{iRq_0}{j_2 \pi \sqrt{4\pi R}} \int_0^{2\pi} e^{-ij_1 z_1(t) - i\frac{j_2 \pi}{R} \sin(t)} (1.5 \sin(t) + 2 \sin(2t)) dt, \quad j_2 \neq 0. \end{aligned}$$

Using, e.g., the composite Simpson's rule, the last integral can be approximated with high order convergence.

Recall that the numbers \hat{u}_j^\pm from (4) were defined to be the Rayleigh coefficients of the scattered

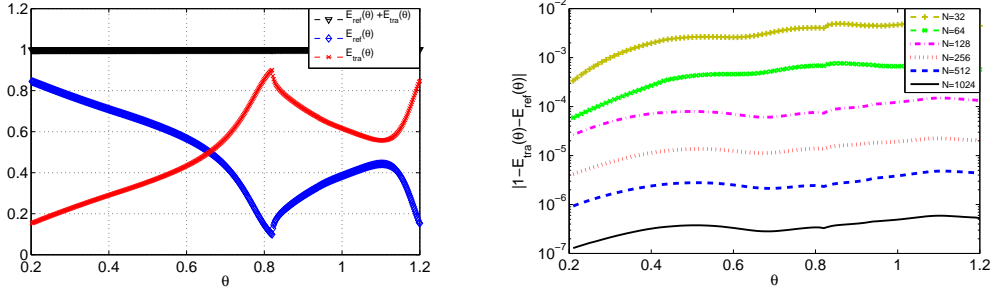


Figure 5: Scattering from periodic kite-shaped structure. (a) Reflected and transmitted energy curves versus the angles θ of the incident field u^i . (b) The error curves $|1 - E_{\text{tra}}(\theta) - E_{\text{ref}}(\theta)|$ for different discretization parameters N versus the angles θ of the incident field u^i .

field. For the incident field, we define similar coefficients by $\hat{u}_j^i = \int_{-\pi}^{\pi} u^i(x_1, -\rho) \exp(-i\alpha_j x_1) dx_1$ for $j \in \mathbb{Z}$. Then Green's formula applied to (2) and the Rayleigh expansion condition show that

$$\sum_{j:k^2 > \beta_j^2} \beta_j (|\hat{u}_j^+|^2 + |\hat{u}_j^- + \hat{u}_j^i|^2) = \beta_0. \quad (59)$$

For an incident wave of direction $(\cos(\theta), -\sin(\theta))^T$, the sums $E_{\text{tra}}(\theta) := \sum_{j:k^2 > \beta_j^2} \beta_j (|\hat{u}_j^- + \hat{u}_j^i|^2) / \beta_0$ and $E_{\text{ref}}(\theta) := \sum_{j:k^2 > \beta_j^2} \beta_j |\hat{u}_j^+|^2 / \beta_0$ correspond to transmitted and reflected wave energies. In this experiment, we use $\theta \mapsto |1 - E_{\text{tra}}(\theta) - E_{\text{ref}}(\theta)|$ as an error indicator for the numerical solution. The wave number k equals π ; further, $\rho = 1$ and $R = 3$. The Rayleigh coefficients of the fields are measured on the line $x_2 = \pm 3/2$. For Figure 5(a) the scattered field is approximated in \mathcal{T}_N where $N = 2^6$. The contrast q equals 5 in D and the tolerance for the GMRES iteration is 10^{-5} . The computation time for solving for one fixed incident angle θ is about 0.8 seconds. In Figure 5(b) we check the energy conservation error for different N . The contrast q for this experiment equals 2 in D and the tolerance for the GMRES iteration is 10^{-10} . As Figure 5(b) shows, the error of the computed Rayleigh coefficients corresponding to propagating modes converges super-algebraically.

A Smoothness of the Difference of Periodic Green's Functions

Lemma A.1. *Assume that $k^2 \neq \alpha_n^2$ for all $n \in \mathbb{Z}$. Then the difference $G_{k,\alpha} - G_{i,\alpha}$ can be written as*

$$G_{k,\alpha}(x) - G_{i,\alpha}(x) = \alpha(|x|^2) + C|x|^2 \ln(|x|) \beta(|x|^2)$$

where α and β are analytic functions and C is a constant.

Proof. Recall that the Bessel function

$$J_n(t) = \sum_{p=0}^{\infty} \frac{(-1)^p}{p!(n+p)!} \left(\frac{t}{2}\right)^{n+2p} \quad n = 0, 1, 2, \dots$$

is an analytic function for all $t \in \mathbb{R}$. It is moreover well-known that the Neumann function

$$Y_n(t) = \frac{2}{\pi} \left\{ \ln \frac{t}{2} + C \right\} J_n(t) - \frac{1}{\pi} \sum_{p=0}^{n-1} \frac{(n-1-p)!}{p!} \left(\frac{2}{t} \right)^{n-2p} \\ - \frac{1}{\pi} \sum_{p=0}^{\infty} \frac{(-1)^p}{p!(n+p)!} \left(\frac{t}{2} \right)^{n+2p} \{ \psi(n+p) + \psi(p) \}$$

is analytic for $t \in (0, \infty)$. (Here $\psi(0) := 0$, $\psi(p) := \sum_{m=1}^p \frac{1}{m}$ for $p = 1, 2, \dots$, and C is Euler's constant.) If $n = 0$ the finite sum in the expression of Y_n is set equal to zero. From [15] we know that the Green's function $G_{k,\alpha}$ can be split as $G_{k,\alpha}(x) = \frac{i}{4} H_0^1(k|x|) + \Psi_k(x)$, where Ψ_k is an analytic function. The same decomposition holds for $G_{i,\alpha}$, with a different analytic function Ψ_i . Hence, it only remains to consider the difference $H_0^1(k|x|) - H_0^1(i|x|)$. To this end, we note that

$$J_0(k|x|) - J_0(i|x|) = \sum_{p=0}^{\infty} \frac{(-1)^p}{(p!)^2 4^p} \left[(k|x|)^{2p} - (i|x|)^{2p} \right] \\ = |x|^2 \sum_{p=0}^{\infty} \frac{(-1)^{p+1}}{[(p+1)!]^2 4^{p+1}} \left[(k)^{2p+2} - (i)^{2p+2} \right] (|x|^2)^p. \quad (60)$$

Use the ratio test one can check that the power series in (60) converges to some analytic function of the variable $|x|^2$ in \mathbb{R} . Moreover, due to the expression of Y_0 we can see that

$$Y_0(k|x|) - Y_0(i|x|) = \frac{2}{\pi} \ln(|x|) \left[J_0(k|x|) - J_0(i|x|) \right] + \Psi_1(|x|^2), \quad (61)$$

where Ψ_1 is an analytic function. Furthermore, we have

$$G_{k,\alpha}(x) - G_{i,\alpha}(x) = \frac{i}{2} \left[H_0^1(k|x|) - H_0^1(i|x|) \right] \\ = J_0(k|x|) - J_0(i|x|) + i \left[Y_0(k|x|) - Y_0(i|x|) \right].$$

Substitution of (60) and (61) into the last equation finishes the proof. \square

Corollary A.2. *Assume that $k^2 \neq \alpha_n^2$ for all $n \in \mathbb{Z}$. Then the difference $L_k - L_i$ is compact on $H_\alpha^1(D)$.*

B Periodic Extension Operators

In this section, we exemplarily show how to construct a periodic extension operator

$$E : H_\alpha^1(D) \rightarrow H_\alpha^1(\Omega), \quad E(u)|_D = u, \quad E(u)|_{\Omega \setminus \Omega_R} = 0,$$

that is used in, e.g., Theorems 4.4 and 5.3. We will only construct E for the case that the boundary of $D = \{(x_1, x_2)^\top : x_1 \in (-\pi, \pi), \zeta_-(x_1) < x_2 < \zeta_+(x_1)\}$ is given by two 2π -periodic Lipschitz continuous functions $\zeta_\pm : \mathbb{R} \rightarrow (-\rho, \rho)$ such that $\zeta_- < -2\rho/3$, $\zeta_+ > 2\rho/3$, and

$$|\zeta_\pm(x_1) - \zeta_\pm(x'_1)| \leq M|x_1 - x'_1|, \quad x_1, x'_1 \in \mathbb{R}.$$

The general case can be tackled using local patches as in [20, Appendix A].

For $u \in H_\alpha^1(D)$, we define

$$v(x_1, x_2) = \begin{cases} u(x_1, 2\zeta_+(x_1) - x_2) & \text{if } \zeta_+(x_1) < x_2 < 2\zeta_+(x_1) - \zeta_-(x_1), \\ u(x_1, x_2) & \text{if } \zeta_-(x_1) < x_2 < \zeta_+(x_1), \\ u(x_1, 2\zeta_-(x_1) - x_2) & \text{if } 2\zeta_-(x_1) - \zeta_+(x_1) < x_2 < \zeta_-(x_1). \end{cases}$$

Note that $2\zeta_+(x_1) - \zeta_-(x_1) > 2\rho$ and that $2\zeta_-(x_1) - \zeta_+(x_1) < -2\rho$. Straightforward computations show that

$$\|v\|_{H^1(\Omega_{2\rho})} \leq \max(\sqrt{3}, 2\sqrt{2}M)\|u\|_{H_\alpha^1(D)},$$

and the definition of v also implies that v is a quasi-periodic function in $H_\alpha^1(\Omega_{2\rho})$.

To define the periodic extension operator, we use a smooth cut-off function $\chi : \mathbb{R} \rightarrow \mathbb{R}$, that satisfies $0 \leq \chi \leq 1$, $\chi(x_2) = 1$ for $|x_2| \leq \rho$, and $\chi(R) = 0$ for $|x_2| \geq R$. Then we set

$$E(v) = w, \quad w(x) = \begin{cases} \chi(x_2)u(x) & \text{for } x \in \Omega_R, \\ 0 & \text{else.} \end{cases}$$

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