Numerical study of high frequency asymptotics of the symbol of the Dirichlet-to-Neumann operator in 2D diffraction problems

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Abstract. A high-frequency asymptotics of the symbol of the Dirichlet-to-Neumann map, treated as a periodic pseudodifferential operator, in 2D diffraction problems is discussed. Numerical results support a conjecture on a universal limit shape of the symbol.

Keywords: Kirchhoff approximation; high-frequency asymptotics; Helmholtz equation; Dirichlet-to-Neumann operator; periodic pseudodifferential operators

1 Introduction

The classical Kirchhoff Approximation (KA) in diffraction theory is an asymptotic relation between the Dirichlet and Neumann data of a solution of an exterior boundary value problem for the Helmholtz equation with frequency parameter $k \gg 1$. The KA is sensitive to the assumption of positive curvature of the boundary and its accuracy deteriorates in the presence of flattening regions [9]. Numerical methods for high-frequency problems have attracted much attention lately – see e.g. [2]. In an attempt to include small and vanishing curvatures uniformly in an asymptotic theory, we propose to study high-frequency asymptotic properties of the Dirichlet-to-Neumann (DtN) operator rather than those of an individual solution. In [5], we conjectured that the pseudodifferential symbol of the DtN operator, appropriately scaled, tends to a simple universal function as $k \to \infty$. Here we report results of a more detailed numerical study. The results support the said conjecture in the case of a convex scatterer. In a non-convex case, we observe a deviation from the universal limit function in a narrow range of it’s argument values.
2 The DtN operator and the Limit Shape Hypothesis

Consider the Helmholtz equation $\Delta u + k^2 u = 0$ in the exterior of a simply connected bounded domain $\Omega \subset \mathbb{R}^2$ with smooth boundary $\Gamma$. Given a function $f$ on $\Gamma$ of a certain regularity $[3, 7]$, the Dirichlet problem $u|_\Gamma = f$ has a unique solution $u$ satisfying the Sommerfeld radiation condition $\partial_r u - iku = o(r^{-1/2})$ as $r \to \infty$. The normal derivative $g = \partial_\nu u|_\Gamma$ is a function of known regularity on $\Gamma$. The map $\mathcal{N} : f \to g$ is called the Dirichlet-to-Neumann (DtN) operator.

Let $s$ be the arclength parameter on $\Gamma$, and $L$ the length of $\Gamma$. Set $\phi = 2\pi s/L$. The Dirichlet and Neumann data $f$ and $g$ in the above diffraction problem are $2\pi$-periodic functions of variable $\phi$. Let $f(\phi) = \sum \hat{f}(n)e^{in\phi}$ be the Fourier series of $f$. Write $\mathcal{N}$ as a periodic pseudodifferential operator (PPDO) $[1, 8]$

$$g(\phi) = \mathcal{N}f(\phi) = \sum_{n=-\infty}^{\infty} \sigma(\phi, n) \hat{f}(n)e^{in\phi}. \quad (1)$$

The function $\sigma(\phi, n) = e^{-in\phi}\mathcal{N}e^{in\phi}$ is called the symbol of $\mathcal{N}$.

The operator $\mathcal{N}$ depends on the boundary $\Gamma$ as well as on the frequency $k$. We reflect this in notation of the symbol by writing $\sigma(\phi, n) = \sigma(\phi, n; k)$. In $[5]$ we noted an universal ($\Gamma$-independent) high-frequency asymptotic behaviour of the symbol as a function of variable $\xi = \xi(n, k) = \frac{2\pi n}{Lk}$. Define

$$\sigma_{\text{lim}}(\xi) = \begin{cases} 
i\sqrt{1-\xi^2}, & |\xi| < 1, \\
-\sqrt{\xi^2-1}, & |\xi| \geq 1. \end{cases}$$

**Hypothesis 1.** For any $\varepsilon > 0$ and any $\xi_* > 1$, there exists $k_* > 0$ such that

$$\left|k^{-1} \sigma(\phi, n; k) - \sigma_{\text{lim}}(\xi(n, k))\right| \leq \varepsilon \quad (2)$$

whenever $k \geq k_*$ and $|\xi(n, k)| \leq \xi_*$.

Here are some theoretical arguments in favour of Hypothesis 1.

1. The statement holds if $\Gamma$ is a circle of any radius $[5]$.

2. If $|\xi(n, k)| > 1$, then the inequality (2) can be established by constructing an asymptotic WKB solution, as pointed out by L. Friedlander (Univ. of Arizona), personal communication, February 2004.
3. A simple if not completely rigorous argument shows that the hypothesis is consistent with KA for a convex domain [5].

Yet we admit that Hypothesis 1 may be true for some classes of boundary curves and false for others. To restore status quo with numerical experiment, we formulate a somewhat weaker Hypothesis 2 below.

Note that the symbol $\sigma_\Gamma(\phi, n; k)$ generally depends on $\phi$ (except when $\Gamma$ is a circle), while the limit function is $\phi$-independent. So we are trying to approximate the DtN operator by a shift-invariant PPDO. It can only be possible if the Fourier series of the symbol in $\phi$ asymptotically reduces to a single constant term. Put (omitting the subscript $\Gamma$ in the right-hand side)

$$
\sigma_\Gamma(\phi, n; k) = \hat{\sigma}_0(n; k) + \hat{\sigma}_{\pm 1}(n; k)e^{\pm i\phi} + \hat{\sigma}_{\pm 2}(n; k)e^{\pm 2i\phi} + \cdots.
$$

(3)

We shall compare the mean symbol $\hat{\sigma}_0(n; k) = (2\pi)^{-1}\int_{0}^{2\pi} \sigma_\Gamma(\phi, n; k) d\phi$ to the limit function and watch whether the $l_2$-norm $||\hat{\sigma}'(n; k)||$ of a bi-infinite vector formed by the rest of Fourier coefficients (3) is relatively small. Recall:

$$
||\hat{\sigma}'(n; k)||^2 = \sum_{m \neq 0} |\hat{\sigma}_m(n; k)|^2.
$$

(4)

**Hypothesis 2.** For any boundary curve $\Gamma$ and any given $\xi_\ast > 1$, $\varepsilon > 0$, and $\delta > 0$, there exists $k_\ast > 0$ such that if $k \geq k_\ast$ and $|\xi(n, k)| \leq \xi_\ast$, then

1. the shape of the mean symbol $\hat{\sigma}_0$ of the DtN operator follows that of $\sigma_{\lim}$:

$$
|k^{-1}\hat{\sigma}_0(\xi(n, k); k) - \sigma_{\lim}(\xi)| \leq \varepsilon;
$$

(5)

2. the remaining Fourier coefficients of the symbol are collectively small:

$$
n^{-1}||\hat{\sigma}'(n, k)|| \leq \varepsilon,
$$

(6)

if distance $(\xi(n, k), I) > \delta$. Here $I$ is either the empty set or a certain “exceptional” set determined by the curve $\Gamma$.

Note that Hypothesis 1 implies Hypothesis 2 with $I = \emptyset$. The parameter $\delta$ in Hypothesis 2 is introduced to account for a non-uniform convergence near $I$ when $I$ is nonempty. Note also that in this paper we require $\Gamma$ to be a smooth curve, but there exist numerical results supporting validity of the statement for domains with corners.
3  Methodology of numerical verification

To test the hypothesis numerically, we use known sample solutions satisfying the Helmholtz equation (HE) in the exterior domain \( \mathbb{R}^2 \setminus \overline{\Omega} \) and the radiation condition (RC), and compute Fourier coefficients of the Dirichlet and Neumann data. Solutions of HE in \( \mathbb{R}^2 \setminus (0, 0) \) with wavenumber \( k \) and satisfying RC are spanned by the Hankel functions \( H_m^{(1)}(kr) \), \( m = 0, 1, \ldots \), \( r = |\vec{r}| = \sqrt{x^2 + y^2} \). The origin can be viewed as an emitter, or source. Now, by taking fictitious sources at arbitrary locations \( \vec{S} \in \Omega \), the family \( H_m^{(1)}(k|\vec{r} - \vec{S}|) \) of sample solutions in \( \mathbb{R}^2 \setminus \overline{\Omega} \) is constructed. For the verification procedure one can use a countable sub-family with linear combinations dense in the space of solutions. In this work, we use \( H_0^{(1)} \)-solutions with sources near the boundary \( \Gamma \) and approximately equidistributed along \( \Gamma \). A possibility to represent an arbitrary solution of HE+RC in the form of a single layer potential (provided \( k^2 \) is not an interior eigenvalue \( \Box \[\text{§3.2.1}] \)), justifies this choice. An extreme opposite possibility is to choose a family of \( H_m^{(1)} \)-solutions, \( m = 0, 1, 2, \ldots \), with fixed source. It needs the Rayleigh hypothesis for domain \( \Omega \) to hold, which is true, for example, if \( \Gamma \) is an ellipse with eccentricity \( e < 1/\sqrt{2} \) [10].

Let us first describe a procedure used in [5]. Take a uniform partition \( \{\vec{P}_l\}, l = 1, 2, \ldots, l_{\text{max}} \) of the curve \( \Gamma \). Evaluate a sample solution \( H_{0}^{(1)}(k|\vec{r} - \vec{S}|) \) and its normal derivative at the points \( \vec{r} = \vec{P}_l \) to obtain the vectors \( f_l \) and \( g_l \) of size \( l_{\text{max}} \). Then compute the discrete Fourier transforms and consider their truncations \( \hat{f}(n), \hat{g}(n), |n| \leq n_{\text{max}} \). Find the ratio \( \tilde{\sigma}(n) = \hat{f}(n)/\hat{g}(n) \) and compare \( k^{-1}\tilde{\sigma}(n) \) to \( \sigma_{\text{lim}} \left( \frac{2\pi n}{Lk} \right) \) to verify Hypothesis 1. Typically in our examples \( Lk \approx 10^2 \div 10^3 \); we chose \( l_{\text{max}} = 2^{12} \div 2^{24} \), and \( n_{\text{max}} \approx 3Lk \). Higher Fourier coefficients are vanishingly small, that is why we cut them off.

In more detail, let \( \vec{r}(\phi), \phi \in [0, 2\pi] \) be the parametrization of \( \Gamma \) by the normalized arclength \( \phi = 2\pi s/L \). Put \( \phi_l = 2\pi l/l_{\text{max}} \) and \( \vec{P}_l = \vec{r}(\phi_l) \). Then

\[
f_l = H_0^{(1)}(k|\vec{r}(\phi_l) - \vec{S}|), \quad g_l = -\varepsilon_l k \left[ 1 - (r'(\phi_l))^2 \right]^{1/2} H_1^{(1)}(k|\vec{r}(\phi_l) - \vec{S}|).
\]

Here \( r(\phi) = |\vec{r}(\phi)| \) and \( \varepsilon_l = (-1)^{p_l} \), where \( p_l \) is the number of intersections of \( \Gamma \) with the open interval \( (SP_l) \). Note that \( p_l \equiv 0 \) and \( \varepsilon_l \equiv 1 \) if \( \Omega \) is convex.

Our judgement about validity of Hypothesis 1 in [5] was based on the outlined procedure, where we effectively kept over the mean symbol \( \tilde{\sigma}_0(n; k) \) only. But this is not enough. Let us engage in the study of components of the vector \( \tilde{\sigma}' \), see [4], — apart from \( \tilde{\sigma}_0(n; k) \). Now we take several sources,
$S_1, \ldots, S_J$ at once. Assume, for the sake of symmetry, that $J$ is odd, \( J = 2m_{\text{max}} + 1 \). Denote by \( f^j_i \) and \( g^j_i \) the data of the solution with source at \( S_j \), and by \( \hat{f}^j(n) \), \( \hat{g}^j(n) \) the corresponding components of the (truncated) discrete Fourier transforms. The following relations follow from (1), (3): for every \( j = 1, \ldots, J \)

\[
\hat{g}^j(n) = \sum_{m} \hat{f}^j(n-m) \hat{\sigma}_m(n-m; k). \tag{7}
\]

Reduce the infinite summation to a finite number of terms keeping only the components \( \hat{\sigma}_m(\cdot; k) \) with \( |m| \leq m_{\text{max}} \). For example, if \( J = 3 \), then for each \( n = -n_{\text{max}}, \ldots, n_{\text{max}} \) after cut-off we get a linear system of three equations with three unknowns \( \hat{\sigma}_0(n; k), \hat{\sigma}_{\pm 1}(n; k) \):

\[
\hat{g}^j(n) = \hat{f}^j(n+1)\hat{\sigma}_{-1}(n+1) + \hat{f}^j(n)\hat{\sigma}_0(n) + \hat{f}^j(n-1)\hat{\sigma}_1(n-1), \quad j = 1, 2, 3.
\]

Solving all obtained systems, we approximately find \( \hat{\sigma}_m(n) \) for (at least) \( |n| \leq n_{\text{max}} - m_{\text{max}} \) and \( |m| \leq m_{\text{max}} \). Now the left-hand sides of the inequalities (5), (6) can be evaluated; of course, summation in (4) is restricted to \( |m| \leq m_{\text{max}} \).

![Figure 1: Test domains: (a) Convex (ellipse), (b) Non-convex (kite [4])](image)

### 4 Results and discussion

We present results for two symmetric domains shown on Fig. 1: the ellipse \( x(t) = \cos t, y(t) = 0.6 \sin t \), and a non-convex “kite” \( x(t) = \cos t + \ldots \)
0.65 \cos 2t - 0.65, \ y(t) = 1.5 \sin t. \ If \ \phi = 0 \ at \ the \ right \ x\text{-}intercept \ of \ \Gamma, \ then \ due \ to \ symmetry \ \hat{\sigma}_m(-n; k) = \hat{\sigma}_{-m}(n, k) \ and \ it \ suffices \ to \ study \ the \ symbols \ for \ n \geq 0.

The real and imaginary parts of the rescaled mean symbol \( k^{-1}\hat{\sigma}_0(n, k) \) are compared to the limit curves on Fig. 2, 3. Here \( \xi = \xi(n, k) \) as defined in Sect. 2. The parameters are: frequency \( k = 200 \); number of sources \( J = 201 \). The kite’s curves exhibit some roughness when \( \xi \in (0.8, 1) \).

Fig. 4 shows the left-hand side of the inequality \( [\ ] \) vs \( \xi(n, k) \) for \( k = 50, 100, 200, 400, 800 \). The value of \( J \) was always set equal to \( k + 1 \). In the case of ellipse, the norm shrinks to naught as \( k \) grows. It isn’t quite so for
the kite. The peak over the interval $(0.8, 1)$ stays steady. In the frameworks of Hypothesis 2, we say that the exceptional set $I$ is empty for the ellipse, though the convergence near $|\xi| = 1$ is much slower than away from $|\xi| = 1$. The set $I$ for the kite is apparently contained in the union $(-1, -0.8) \cup (0.8, 1)$.

**Computational note.** Computation of the Fourier coefficients $\hat{\sigma}_m(n; k)$ of the symbol requires solution of truncated systems (7). If the cutoff subscript is rather large, one has to take trouble to ensure that Fourier coefficients $\hat{f}(n - m)$ are not vanishingly small. To this end, the sources should be placed close to the boundary, preventing the Dirichlet data of sample solutions from being “too smooth”. The reported results are obtained with sources located at the distance from about $10^{-2}$ to $10^{-3}$ (for larger values of $k$) from $\Gamma$.

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