Symbol of the Dirichlet-to-Neumann operator in 2D diffraction problems with large wavenumber

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Consider the Dirichlet-to-Neumann operator $\mathcal{N}$ in the exterior problem for the 2D Helmholtz equation outside a bounded domain with smooth boundary. Using parametrization of the boundary by normalized arclength, we treat $\mathcal{N}$ as a pseudodifferential operator on the unit circle. We study its discrete symbol.

We put forward a conjecture on the universal behaviour, independent of shape and curvature of the boundary, of the symbol as the wavenumber $k \to \infty$. The conjecture is motivated by an explicit formula for circular boundary, and confirmed numerically for other shapes. It also agrees, on a physical level of rigor, with Kirchhoff’s approximation. The conjecture, if true, opens new ways in numerical analysis of diffraction in the range of moderately high frequencies.

INTRODUCTION

This work is a part of research aimed at an accurate and robust numerical algorithm for diffraction problems in mid-high frequency range, where the standard Boundary Integral Equation methods fail due to large matrix size and, more importantly, to numerical contamination in quadratures. A natural idea to use the knowledge of geometric phase and to separate fast oscillations from slowly varying amplitudes has been converted to a practical method \cite{1,2} with recent enhancements \cite{7}. A drawback of that approach occurs in the presence of flattening boundary regions, where Kirchhoff’s amplitude becomes singular. From numerical analyst’s point of view, a method that has problem with small curvature is anti-intuitive.

The point of our approach is to look for an object in theory whose high-frequency asymptotics stands flattening well and isn’t sensitive to convexity assumptions. We suggest that the symbol of Dirichlet-to-Neumann operator might be such an object.

We consider the 2D case and don’t claim a ready-made extension of our results in 3D. As a technical reason, we need a well defined full symbol of a pseudodifferential operator on a compact manifold (the boundary). In the 2D case, the boundary is a closed curve, so a special version of the PDO theory with discrete frequency variable is applicable, which attends to smooth kernels and doesn’t require partitions of unity.

DIRICHLET-TO-NEUMANN OPERATOR

Let $\Omega$ be a bounded domain in $\mathbb{R}^2$ with smooth boundary $\Gamma$. The exterior Dirichlet problem for the Helmholtz equation in polar coordinates $r, \phi$ reads
\[ \Delta u \equiv \frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} + \frac{1}{r^2} \frac{\partial^2 u}{\partial \phi^2} = -k^2 u \quad \text{in} \quad \mathbb{R}^2 \setminus \bar{\Omega}, \]

\[ \frac{\partial u}{\partial r} - iku = o(r^{-1/2}), \quad r \to \infty, \]

\[ u|_{\Gamma} = f. \quad (1) \]

For a function \( f \in C^1(\Gamma) \), the problem has unique solution \( u \), and its normal derivative \( g = \partial_n u|_{\Gamma} \) is a continuous function on \( \Gamma \). (For sharper conditions see e.g. [5], [10].) The map \( \mathcal{N} : f \to g \) is called the \textit{Dirichlet-to-Neumann operator} for Problem (1).

**Operator \( \mathcal{N} \) for the exterior of the unit disc**

Here the boundary is the unit circle \( S \) and it can be parametrized by \( \phi \). Consider Fourier series of the \( 2\pi \)-periodic functions \( f(\phi) = u|_S \) and \( g(\phi) = \partial_n u|_S \)

\[ f(\phi) = \sum_{n \in \mathbb{Z}} \hat{f}(n)e^{in\phi}, \quad g(\phi) = \sum_{n \in \mathbb{Z}} \hat{g}(n)e^{in\phi}. \]

The Helmholtz equation has outgoing elementary solutions in the product form

\[ e^{in\phi} H^{(1)}_{|n|}(kr), \]

where \( H^{(1)}_{|n|} \) are Hankel functions [8] (9.1.3). The solution \( u(r, \phi) \) can be represented as a linear combination of the elementary solutions. Matching Fourier coefficients in the boundary data, we find

\[ \hat{g}(n) = \sigma(n; k) \hat{f}(n), \]

where (cf. [8] (9.1.27.4) )

\[ \sigma(n; k) = k \frac{\partial_k H^{(1)}_{|n|}(k)}{H^{(1)}_{|n|}(k)} = -k \frac{H^{(1)}_{|n|+1}(k)}{H^{(1)}_{|n|}(k)} + |n|. \quad (2) \]

The operator \( \mathcal{N} \) can be written in a pseudodifferential fashion, the function \( \sigma \) being its \textit{discrete symbol} (here dependence of \( \sigma \) on the wavenumber \( k \) is irrelevant and is omitted)

\[ \mathcal{N} f(\phi) = \sum_{n \in \mathbb{Z}} \sigma(n) \hat{f}(n) e^{in\phi}. \quad (3) \]

**Asymptotics of the symbol**

For a fixed \( k \) and \( n \to \infty \), we derive from [8] (9.3.1)

\[ \frac{H^{(1)}_{n+1}(k)}{H^{(1)}_{n}(k)} \sim \frac{2n}{k}, \]

so (in full agreement with pseudodifferential calculus)

\[ \sigma(n; k) \sim -|n|, \quad |n| \to \infty. \quad (4) \]
On the other hand, if \( n \) is fixed, then by [8] (9.2.3)

\[
\sigma(n; k) \sim ik, \quad k \to \infty.
\]  

(5)

The next result, in which the ratio \( t = n/k \) is fixed, interpolates between the above two special cases. Since \( n \) is an integer, the integral part function \([\cdot]\) is involved.

**Lemma.** For any fixed \( t \geq 0 \) and \( n = n(k,t) = \lfloor kt \rfloor \),

\[
\lim_{k \to \infty} \frac{\sigma(n; k)}{k} = \sigma_{\text{lim}}(t) = \begin{cases} 
  i\sqrt{1-t^2}, & \text{if } t \leq 1 \\
  -\sqrt{t^2-1}, & \text{if } t \geq 1
\end{cases}
\]  

(6)

This fact can be derived laboriously using [8] (9.3.37–46) and asymptotics for the Airy functions. Instead, we demonstrate a simple argument, which quickly produces the formula in the case \( t \neq 1 \), and can be converted to a formal proof.

Consider a recurrence for the ratios \( \mu_\nu \) of Hankel functions of orders \( \nu + 1 \) and \( \nu \) with fixed argument \( k \). According to [8] (9.1.27.1), we have

\[
\mu_\nu + \mu_{\nu-1}^{-1} = 2\nu/k,
\]

or in the explicit difference form,

\[
\mu_\nu - \mu_{\nu-1} = -\mu_{\nu-1} - \mu_{\nu-1}^{-1} + 2t_\nu, \quad t_\nu = \nu/k.
\]  

(7)

The ratio \( t_\nu \) varies slowly. Consider the difference equation with \( \nu \sim n \) and frozen \( t_\nu = t_n = t \). It has two complex stationary solutions

\[
\mu^\pm = t \pm \sqrt{t^2 - 1}.
\]  

(8)

The equation in variations for (7) is

\[
\delta \mu_\nu - \delta \mu_{\nu-1} = (-1 + \mu_{\nu-1}^{-2}) \delta \mu_{\nu-1}.
\]

Therefore, for \( 0 < t < 1 \) both solutions [8] are asymptotically stable, while for \( t > 1 \) the solution \( \mu^+ \) is asymptotically stable, and \( \mu^- \) unstable. A solution of the equation with frozen \( t_\nu \) approaches its limit exponentially fast, so the value of \( \nu \) near \( n \) doesn’t change significantly while the stabilization occurs. Since by (2)

\[
\sigma(n; k) = k (-\mu_n + t),
\]

and the attractor \( \mu^+ \) is unique in the case \( t > 1 \), we immediately obtain (6) in that case. In the case \( 0 < t < 1 \), the solution \( \mu_\nu \) approaches \( \mu^- \) with negative imaginary part, because the initial value \( \mu_0 \approx -i \), cf. (3).

**Note.** The Lemma holds for \( t = 1 \) due to the asymptotics derived from [8] (9.3.31–34)

\[
\frac{\partial_k H^{(1)}_k(k)}{H^{(1)}_k(k)} \sim 6^{1/3} \frac{(1+i\sqrt{3})\Gamma(2/3)}{(1-i\sqrt{3})\Gamma(1/3)}, \quad k \to \infty.
\]
Disc of arbitrary radius

Let \( u(r, \phi; R, k) \) be a solution of Problem (1) with wavenumber \( k \) outside a circle of radius \( R \). Then \( u(r/R, \phi; 1, kR) \) is a solution of Problem (1) with wavenumber \( kR \) outside the unit circle. The Dirichlet data for the two functions (as functions of \( \phi \)) are identical, \( f_{R,k}(\phi) = f_{1,kR}(\phi) \). The Neumann data are related via

\[
g_{R,k}(\phi) = \partial_r u(r, \phi; R, k) \big|_{r=R} = R^{-1} g_{1,kR}(\phi).
\]

Correspondingly, the symbol of the operator \( \mathcal{N} \) for the disk of radius \( R \) is

\[
\sigma_R(n, k) = R^{-1} \sigma_1(n, kR), \tag{9}
\]

so the limit formula \( 6 \) of Lemma holds with \( n = n(k, t) = [kRt] \). Equivalently, we can write the argument of the limit function \( \sigma_{\text{lim}}(t) \) as

\[
t = \frac{n}{kR} = \frac{2\pi n}{L} \frac{n}{k}, \tag{10}
\]

where \( L = 2\pi R \) is the circumference of the boundary. Notice that the factor \( 2\pi/L \) is the Jacobian \( \partial \phi/\partial s \) of the boundary parameter change from the arclength \( s \) to \( \phi \).

In the limit \( R \to \infty \) the disk becomes a half-plane and an analog of the asymptotic formula \( 6 \) is an exact formula \( 12 \) below.

Half-plane

For the Helmholtz equation in the half-plane \((x \in \mathbb{R}, y > 0)\), Sommerfeld’s radiation condition is replaced by a condition that explicitly specifies allowed harmonics in the decomposition of any outgoing solution. Namely, two differently behaved families of elementary outgoing solutions are given by

\[
w(x, y; \xi) = \begin{cases} 
  \exp\{ix\xi + iy\sqrt{k^2 - \xi^2}\}, & -1 < \xi < 1, \\
  \exp(ix\xi) \exp(-y\sqrt{\xi^2 - k^2}), & |\xi| > 1.
\end{cases}
\]

The general outgoing solution has the form

\[
u(x, y) = \int_{-\infty}^{\infty} \hat{f}(\xi) w(x, y; \xi) d\xi, \tag{11}
\]

(we don’t discuss possible classes to which the function \( \hat{f}(\xi) \) may belong).

It is readily seen that \( \hat{f}(\xi) \) is the Fourier transform of the Dirichlet boundary data \( f(x) = u(x, 0) \). Differentiating \( 11 \) with respect to \( y \), we obtain the Fourier representation for the Neumann data \( g(x) \). The formula for the Dirichlet-to-Neumann operator, an analog of \( 3 \), reads

\[
\mathcal{N} f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \sigma(\xi) \hat{f}(\xi) e^{ix\xi} d\xi,
\]

where the symbol \( \sigma(\xi) = \sigma(\xi; k) \) is \( \partial_y w(x, y; \xi)/w(x, y; \xi)|_{y=0} \), i.e.

\[
\sigma(\xi; k) = k \sigma_{\text{lim}}(\xi/k). \tag{12}
\]
The reader can probably see what conclusion we are about to draw from the above examples. Let us complete technical preparations, then formulate the main conjecture.

Recall briefly and informally some basic notions regarding pseudodifferential operators on the unit circle $S$. See [3], [11] for a full account of the topic.

Let $a(\phi, n)$ be a function on $S \times \mathbb{Z}$, which satisfies certain regularity conditions. The function $a(\phi, n)$ is the discrete symbol of the periodic pseudodifferential operator (PPDO) $A$ defined by the formula

$$Af(\phi) = \sum_{n \in \mathbb{Z}} a(\phi, n) \hat{f}(n)e^{in\phi}.$$  

Here $f(\phi)$ is a $2\pi$-periodic function and $\hat{f}(n)$ its Fourier coefficients.

The symbol $\sigma(n)$ introduced in (3) does not depend on $\phi$. Such symbols are called constant symbols, and corresponding operators are shift invariant.

The theory of PPDO applies not only to operators on the unit circle, but to operators on any smooth closed curve, since functions on closed curved can be identified with $2\pi$-periodic functions by reparametrization.

The symbol $a(\phi, n)$ of a PPDO $A$ typically has an asymptotic expansion in decreasing powers of $n$. The principal symbol is the leading term in the asymptotics

$$a(\phi, \pm|n|) = a_0^\pm(\phi)|n|^\alpha + o(|n|^\alpha), \quad |n| \to \infty,$$

and $\alpha$ is the order of $A$. For example, for any domain the operator $N$ is a PPDO of order of 1, and for the unit disk its principal symbol is $-|n|$, cf. (4).

Theory of PPDO is somewhat simpler than the general theory of pseudodifferential operators on compact manifolds (see e.g. [12]). The definition of a general PDO uses partition of unity. Only the principal symbol can be defined globally.

The discrete symbol $a(\phi, n)$ of a classical PPDO agrees on $\mathbb{Z}$ with a symbol $\tilde{a}(\phi, \xi)$ defined in the general theory, modulo a function with asymptotics $O(|n|^{-\infty})$.

Reconstruction of an operator by its symbol in the general theory assumes that operators with smooth kernels are neglected. It isn’t convenient when one studies double asymptotics (in $\xi$ and $k$), since the behaviour of the neglected part with respect to $k$ is not controlled. Correspondence between operators and symbols in the theory of PPDO with discrete symbols is strict and preserves full information in both directions.

**Limit Shape Conjecture**

We return to Problem 1 with general boundary $\Gamma$. Denote the length of $\Gamma$ by $L$. Let $s$ be the arclength parameter on $\Gamma$ (with an arbitrarily chosen starting point), and set

$$\psi = s \frac{2\pi}{L}, \quad 0 \leq \psi < 2\pi.$$  

Consider the operator $N$ as a PPDO (with respect to the parametrization by $\psi$). Denote its symbol as $\sigma_{\Gamma}(\psi, n; k)$, emphasizing dependence on the wavenumber $k$. 

Conjecture. For any fixed \( t \in \mathbb{R} \) and \( n = n(k, t) = [(L/2\pi)kt] \), there exists

\[
\lim_{k \to \infty} \frac{\sigma(\psi, n; k)}{k} = \sigma_{\lim}(t).
\]

uniformly w.r.t. \( \psi \). The universal function \( \sigma_{\lim}(t) \) is defined in (6).

Let us say less formally:

\[
\sigma(\psi, n; k) \approx k \sigma_{\lim}\left(\frac{2\pi n}{L}k\right).
\]

We can make the conjecture even more readable at the expense of precise mathematical meaning. Let us ignore problems associated with definition of a global symbol of PDO in the standard theory, where the frequency argument is continuous. Assume that \( \sigma(s, \xi; k) \) is the symbol of the operator \( \mathcal{N} \) corresponding to the arclength parametrization of the boundary. Then

\[
\sigma(s, \xi; k) \approx \begin{cases} 
  i\sqrt{k^2 - \xi^2}, & \xi < k \\
  -\sqrt{\xi^2 - k^2}, & \xi > k.
\end{cases}
\]

Thus the symbol for any boundary parametrized by the arclength is asymptotically equal to the exact symbol for the half-plane. This conclusion is hardly surprising given that at high frequencies the diffraction process is well localized and (13) takes place for any disc — see (6), (10) — and doesn’t refer to curvature.

Our conjecture has no problems with tangent rays and shadow regions since the formula doesn’t depend on the boundary data. In particular — in the case of a plane incident wave — the direction of incidence has no effect on our claim. One can argue that the conjecture has no backing in the case of non-convex scatterers. In that case it is supported by numerical results; see the last section of the paper.

Kirchhoff’s approximation

A relation between the boundary data \( f \) and \( g \) of an outgoing solution can be described alternatively by the impedance function \( \eta = g/f \). It depends on the solution. However, according to Kirchhoff’s approximation, at high frequencies the impedance function approaches an universal function that depends only on the boundary shape. Let us ”derive” this approximation from the Conjecture.

Consider an incident plane wave \( u_{\text{inc}} \) with the wave vector \( kk_0, \|k_0\| = 1 \). Let \( n \) be the unit normal vector to the boundary \( \Gamma \) at the given point \( P \in \Gamma \). Denote by \( \theta \) the angle between \( k_0 \) and \( n \) (Fig. 1). The incident wave length \( \lambda = 2\pi/k \) is the
distance between wave fronts with equal phases. The boundary value \( u_{\text{inc}}|_{\Gamma} \) oscillates with period \( \Lambda = \lambda / \sin \theta \) near the point \( P \). We say that local frequency of \( u_{\text{inc}}|_{\Gamma} \) at \( P \) is \( \xi = 2\pi / \Lambda = k \sin \theta \). Assuming Dirichlet’s condition for the total field \( u_{\text{inc}} + u \) the boundary value \( f = u_{\Gamma} \) also oscillates with local frequency \( \xi \) at \( P \).

From a physical point of view, the action of the operator \( \mathcal{N} \) amounts to multiplication of local Fourier harmonics by the values of the symbol \( \sigma_{\Gamma} \) at corresponding space-frequency locations. In the present case, where the harmonic with frequency \( \xi \) dominates at point \( P \), formula (13) implies

\[
\mathcal{N} u(P) \approx \sigma_{\Gamma}(P, \xi; k) u(P) \approx i \sqrt{k^2 - \xi^2} u(P) = ik \cos \theta u(P).
\]

(14)

Fig. 1 shows an illuminated region of the boundary, but the argument holds for a shadow region as well. Formula (14) can be written in the form

\[
\eta(P) \approx ik |\langle \mathbf{k}_0, \mathbf{n}(P) \rangle|,
\]

which is the classical Kirchhoff approximation formula [9]. A rigorous mathematical treatment of Kirchhoff’s approximation (for convex domains) is given in [12, Ch. X].

**Insufficiency of the naive local frequency analysis**

The simplistic understanding of the symbol via local frequencies fails in the following example. Consider the horse-shoe domain \( \Omega \) as shown on Fig. 2. Let two solutions \( u^{(1)} \) and \( u^{(2)} \) of Problem (11) be defined outside \( \Omega \) as cylindrical waves generated by the fictitious sources at the points \( S_j \), \( j = 1, 2 \), inside \( \Omega \). From asymptotics of Hankel’s function \( H_0^{(1)}(kr) \) we see that if \( k|S_j P| \gg 1 \), then the two solutions yield opposite impedances \( \eta_1(P) \approx -\eta_2(P) \approx -ik \).

The local tangential frequency at \( P \) is close to 0 for both solutions. Thus it is impossible to determine the value \( \sigma_{\Gamma}(P, 0; k) \) consistently by this approach.

**Numerical verification of the Conjecture**

The following algorithm has been used to retrieve the symbol of the operator \( \mathcal{N} \). Assume \( k \) is given. The algorithm has three free parameters: number of nodes \( N \) (taken in the form \( N = 2^m \) for convenience), and coordinates \((x_S, y_S)\) of a fictitious source inside the domain \( \Omega \).
Algorithm.

1. Find an equidistant partition of $\Gamma$ by $N$ nodes $P_i$.

2. Boundary data will be taken from the sample outgoing solution

$$u(P) = H_0^{(1)}(k|PS|), \quad P \notin \Omega,$$

where $S = (x_S, y_S)$ is the "source", and $P$ is an observation point. Compute the boundary data $f_i = u(P_i), \ g_i = \partial_n u(P_i), \ i = 1, \ldots, N$.

3. Compute discrete Fourier transforms $\hat{f}(n), \ \hat{g}(n), \ n = 0, \ldots, N - 1$, of the arrays $\{f_i\}, \ \{g_i\}$ using FFT algorithm. Only the first $n_{\text{max}}$ Fourier coefficients are considered reliable and are used in the sequel.

4. Find the truncated symbol of a shift-invariant operator that takes $f$ to $g$:

$$\tilde{\sigma}(n) = \frac{\hat{g}(n)}{\hat{f}(n)}, \quad n = 0, \ldots, n_{\text{max}} - 1.$$

5. To verify the Conjecture, compare the values $k^{-1}\tilde{\sigma}(n)$ to $\sigma_{\text{lim}}(2\pi n/kL)$, where $L$ is the length of $\Gamma$.

We present results obtained for the kite domain [6, p. 70] shown on Fig. 3 and defined by the parametric equations

$$x(t) = \cos t + 0.65 \cos 2t - 0.65, \quad y(t) = 1.5 \sin t, \quad t = 0 \ldots 2\pi.$$ 

![Fig. 3: Test domain ("kite")](image)

The parameters are: $k = 200, \ N = 2^{20}, \ S(-0.7, 0.5)$. The width of the triangle on Fig. 3 is equal to 10 wavelengths. In this example, length $L = 9.32402$ and $kL/2\pi \approx 297$.

On Fig. 4, the horizontal coordinate is $t = 2\pi n/kL$. Thick lines show the normalized real (a), with negative sign, and imaginary (b) parts of the computed approximate
symbol, $k^{-1} \tilde{\sigma}(n)$. Thin lines are the conjectured limit shapes. The true symbol $\sigma_\Gamma$ in this case is non-constant, so the approximation by a shift-invariant symbol depends on the chosen position of the source. For a source closer to the center of the kite, oscillations near $t = 1$ become smaller. However, in that case the computed values near $t = 2$ oscillate wildly, because corresponding Fourier coefficients $\hat{f}(n)$ become evanescent.

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{symbol-plot.png}
\caption{Computed symbol $k^{-1} \tilde{\sigma}(n)$ vs $\sigma_{\text{lim}}(t)$, $t = \frac{2\pi}{kL} n$}
\end{figure}

The upper bound $t_{\text{max}} \approx 2.3$ on the graphs corresponds to $n_{\text{max}} = 700$ set in the computer program. Stabilization of the Fourier coefficients at the upper end of this range occurs for the order of discretization $N \geq 2^{18}$. Obtaining stable values of the approximate symbol at larger values of $t$ requires use of larger values of $N$ that grow, roughly, exponentially with $t$.

A program used for these calculations had a 12 byte long type for floating point operations (long double in C). The results obtained with a 8 byte long arithmetics (C’s type double) were nearly identical. So in the considered example numerical errors due to a limited precision are not an issue.

\section*{Conclusion}

The main result is the proposed Limit Shape Formula (13) for the symbol of the Dirichlet-to-Neumann operator for the standard 2D diffraction problem (1) with smooth boundary. This asymptotics is independent of the boundary data, of the boundary curvature, and of convexity assumptions. The limit function $\sigma_{\text{lim}}(t)$ defined in (6) varies slowly in its argument $t \sim \text{const} \, n/k$, except near $t = 1$. These features make the approximation (13) useful for numerical completion of the boundary data set $(u|_\Gamma, \partial_n u|_\Gamma)$, which yields the solution $u$ and the radiation pattern by Green’s formula. This approach includes and supersedes the classical Kirchhoff approximation. We believe that
the asymptotics can be enhanced and next, curvature-dependent, term(s) can be found from the theory of pseudodifferential operators. In the especially important region, a narrow neighbourhood of $t = 1$, methods for a field near a caustic \[ \] can be used.

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