Diffraction Effects in the Scattering of Waves

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Abstract. This paper describes the use of parametrices for diffractive boundary value problems in the study of effects of grazing rays on the behavior of scattered waves. It is a TeXed version of the paper [T6], with updated references.

Introduction

This paper summarizes a number of developments in the study of diffractive boundary value problems made during the period 1975–81. In the first two sections, work of Melrose [Mel1], [Mel3] and Taylor [T1], [T4] on the construction of parametrices for such a grazing ray problem are reviewed. We restrict attention to the Dirichlet problem for the usual scalar wave equation. In Sections 3–5 we sketch some joint work of Melrose and Taylor [MeT] on Fourier integral operators with folding canonical relations, and applications to some problems in scattering theory, and on the corrected Kirchhoff approximation. Section 6 describes some results of Farris [F2] on the solution operator to the wave equation with diffractive boundary.

Throughout this paper, we make use of pseudodifferential operators with symbols $p(x,\xi)$ in the class $S^m_{\rho,\delta}$ of Hörmander [H1], i.e., satisfying estimates

$$|D_x^\beta D_\xi^\alpha p(x,\xi)| \le C_{\alpha\beta}(1+|\xi|)^{m-\rho|\alpha|+\delta|\beta|}.$$

A subclass of $S^m_{1,0}$ is S^m, consisting of $p(x,\xi)$ asymptotic to $\sum_{j\ge 0} p_{m-j}(x,\xi)$, with $p_{m-j}(x,\xi)$ homogeneous of degree $m-j$ in ξ, for $|\xi|\ge 1$. Also, we say $p(x,\xi,\eta)\in \mathcal{N}^m_\rho$ provided

$$|D_x^\beta D_\xi^\alpha D_\eta^j p(x,\xi,\eta)| \le C_{\beta\alpha j}|\xi|^{m-|\alpha|}(|\xi|^\rho+|\eta|)^{-j}.$$

This paper originally appeared as [T6]. The current version (in TeX, rather than off an old fashioned typewriter) makes few changes to that original, other than updating references and fixing some typos. (There are corrections to (5.14) and (5.19).) The paper [T6] had two additional sections (§§7–8), dealing with systems of wave equations, which are omitted here.

We mention the monograph [MeT2], which discusses parametrix construction for wave equations, in both the grazing and the gliding ray contexts, which was produced after [T6]. (Chapters 11–12 of [MeT2] cover material on systems of wave equations omitted from this version of [T6].)

In this paper we make no mention of non smooth obstacles. For a study of diffraction of waves by cones and polyhedra, see [CT], which is summarized in [T5], and also in Chapter 8, §8, of [T8].

1. The grazing ray parametrix

In this section we review the construction of a parametrix for the solution of the wave equation on the exterior of a convex domain $K \subset \mathbb{R}^n$, assumed to be smooth, with strictly positive curvature. Such parametrices were constructed in [Mel1] and [T1]; see also [Mel3] and [T4]. We briefly discuss some refinements (also treated in the monograph [MeT2]).

We look for a parametrix for the solution to the problem

$$\begin{aligned}
&(1.1) && \Big(\frac{\partial^2}{\partial t^2} - \Delta\Big) u = 0 \quad \text{on} \quad \mathbb{R}^n \setminus K, \\
&(1.2) && u\big|_{\mathbb{R}\times\partial K} = f, \\
&(1.3) && u = 0 \quad \text{for} \quad t << 0,
\end{aligned}$$

given $f \in \mathcal{E}'(\mathbb{R} \times \partial K)$. The boundary condition (1.2) is the Dirichlet boundary condition. Also of interest is the Neumann boundary condition

$$\frac{\partial u}{\partial \nu}\Big|_{\mathbb{R}\times\partial K} = g. \tag{1.4}$$

This, and a large class of other boundary conditions, is amenable to treatment, given the discussion of the Neumann operator which we will provide in Section 2.

We will assume $\mathrm{WF}(f)$ is contained in a small conic neighborhood of a point in $T^*(\mathbb{R} \times \partial K)$ over which a grazing ray passes, since the non-grazing case is relatively elementary. The parametrix we will construct is of the form

$$u(t,x) = \iint \Big(g \frac{A(\xi_1^{-1/3}\rho)}{A(-\xi_1^{-1/3}\eta)} + ih\xi_1^{-1/3} \frac{A'(\xi_1^{-1/3}\rho)}{A(-\xi_1^{-1/3}\eta)} \Big) e^{i\theta} \hat{F}(\xi,\eta)\, d\xi\, d\eta. \tag{1.5}$$

The phase functions ρ, θ will solve certain eikonal equations and the amplitudes g, h will solve certain transport equations.

The function $A(s) = A_\pm(s)$ is a certain Airy function, $A_\pm(s) = Ai(e^{\pm(2/3)\pi i}s)$, solving the Airy equation $A''(s) - sA(s) = 0$. $A(s)$ blows up as $s \to +\infty$ and is oscillatory as $s \to -\infty$. In fact, one has

$$A_\pm(s) = \pm\frac{i}{2}e^{\mp(2/3)\pi i}F(s)e^{\mp i\chi(s)}, \tag{1.6}$$

where $F(s)^{-1} \in S^{1/4}_{1,0}(\mathbb{R})$, $\chi(s) \in S^{3/2}_{1,0}(\mathbb{R})$ have expressions of the form

$$\begin{aligned} F(s)^2 &\sim \frac{1}{\pi\sqrt{-s}}\Big[1 - a_1(-s)^{-3/2} + \cdots\Big], \quad \text{as} \quad s \to -\infty, \\ F(s) &\sim \frac{1}{\pi}e^{(2/3)s^{3/2}}, \quad \text{as} \quad s \to +\infty, \\ \chi(s) - \frac{\pi}{4} &\sim \frac{2}{3}(-s)^{3/2}\Big[1 - b_1(-s)^{-3/2} + \cdots\Big], \quad \text{as} \quad s \to -\infty. \end{aligned}$$

χ is real, and $\chi'(s) = -1/\pi F(s)^2$. Background material on the Airy function can be found in [Mil], and in Appendix A of [MeT2].

It turns out that we can find solutions to the eikonal equations

$$\begin{aligned} \theta_t^2 - |\nabla_x\theta|^2 + \frac{\rho}{\xi_1}(\rho_t^2 - |\nabla_x\rho|^2) &= 0, \\ \theta_t\rho_t - \nabla_x\theta\cdot\nabla_x\rho &= 0, \end{aligned} \tag{1.7}$$

on $\mathbb{R}^n \setminus K$ for $\eta \ge 0$, and to infinite order on ∂K for $\eta \le 0$, such that

$$\rho\Big|_{\mathbb{R}\times\partial K} = -\eta, \tag{1.8}$$

and such that

$$\frac{\partial\rho}{\partial\nu}\Big|_{\mathbb{R}\times\partial K} < 0. \tag{1.9}$$

(The functions ρ, θ are real valued, smooth, and homogeneous of degree 1 in (ξ, η).) From this, the asymptotic relation (1.6) makes sense out of (1.5) as a Fourier integral operator with singular phase function. The unknown distribution F, with wave front set in a small conic neighborhood of $\{\eta = 0\}$, is related to $u|_{\mathbb{R}\times\partial K} = f$ by a Fourier integral operator. Indeed, using (1.8) and the similarly derived fact that one can arrange

$$h\Big|_{\mathbb{R}\times\partial K} = 0, \tag{1.10}$$

one gets, with $\theta_0 = \theta|_{\mathbb{R}\times\partial K}$,

$$u\Big|_{\mathbb{R}\times\partial K} = \iint g e^{i\theta_0}\hat{F}\,d\xi\,d\eta = JF. \tag{1.11}$$

In solving the transport equation for g one can arrange that g be nonvanishing on a small conic set, and the phase function θ_0 can be seen to yield a non-degenerate canonical transformation $\mathcal{J}$, so J is an elliptic Fourier integral operator, and hence is microlocally invertible. Thus, the parametrix to (1.1)–(1.3) is given by (1.5) with

$$F = J^{-1} f. \tag{1.12}$$

We briefly go over the solution to the eikonal equation (1.7), satisfying the condition (1.8), which is more restrictive than the condition

$$\rho\big|_{\mathbb{R}\times\partial K} = -\eta + O\Big(|\xi|\Big(\frac{|\eta|}{|\xi|}\Big)^{\infty}\Big),$$

proved and used in [T1] and [T4]. The extra ingredient used to obtain (1.8) is Melrose's result on equivalence of glancing hypersurfaces [Mel2]. Melrose [Mel3] has noted that this result leads to solutions to (1.7) such that $\rho|_{\mathbb{R}\times\partial K}$ is independent of (t, x). The argument we sketch here is just a little different from that one.

Let $\Omega = \mathbb{R} \times (\mathbb{R}^n \setminus K)$. The pair of hypersurfaces $J_1 = T^*_{\partial\Omega}(\mathbb{R}^{n+1})$ and $K_1 = \{|\xi|^2 - \tau^2 = 0\}$ in $T^*(\mathbb{R}^{n+1})$ has glancing intersection, in the sense of [Mel2]. Consequently, there is a (microlocally defined) homogeneous symplectic map

$$T^*(\mathbb{R}^{n+1}_+) \xrightarrow{\chi} T^*\Omega, \tag{1.13}$$

taking the "canonical pair" of hypersurfaces to J_1, K_1. More precisely, $J_0 = \{x_{n+1} = 0\}$ is taken to J_1 and $K_0 = \{p_0(x, \xi) = 0\}$ is taken to K_1 by χ, where

$$p_0(x, \xi) = \xi_{n+1}^2 - x_{n+1}\xi_1^2 + \xi_1\xi_n. \tag{1.14}$$

Now, on J_1 and J_0, the symplectic form gives a Hamilton foliation. Let this determine an equivalence relation $\sim$. Then $J_1 \cap K_1/\sim$ has the structure of a symplectic manifold with boundary, and is naturally isomorphic to the closure of the "hyperbolic" region in $T^*(\partial\Omega)$, the region over which real rays pass, and similarly $J_0 \cap K_0$ is naturally isomorphic to the closure of the hyperbolic region in $T^*(\partial\mathbb{R}^{n+1}_+)$. Thus we get a homogeneous symplectic map

$$T^*(\partial\mathbb{R}^{n+1}_+) \xrightarrow{\chi_J} T^*(\partial\Omega), \tag{1.15}$$

defined in the hyperbolic regions, smooth up to the boundary, which consists of the grazing directions. Furthermore, χ_J intertwines the "billiard ball maps" $\delta_0^{\pm}$ and $\delta^{\pm}$. Here, the billiard ball maps $\delta^{\pm} : T^*(\partial\Omega) \to T^*(\partial\Omega)$, defined on the hyperbolic region, continuous up to the boundary, smooth in the interior, are defined at a point (x_0, ξ_0) by taking the two rays that lie over this point, in the variety $K_1 = \{|\xi|^2 - \tau^2 = 0\}$, and following the null bicharacteristics through these points until you pass over $\partial\Omega$ again, projecting such a point onto $T^*(\partial\Omega)$; δ^+ increases the t-coordinate and δ^- decreases it. $\delta_0^{\pm}$ is defined similarly.

Let $v \in \Lambda'(\partial\Omega)$ be a gradient field corresponding under χ_J to some $(\xi_1, \dots, \xi_n) =$ const. in $T^*(\mathbb{R}^n)$. Let $S_v \subset T^*\Omega$ be the Hamilton flow-out, where $S_v|_{\partial\Omega}$ is identified with the appropriate point in $K_1 \subset T^*\Omega$ lying over $v \in T^*(\partial\Omega)$. Let $S_\xi \subset T^*\mathbb{R}^{n+1}$ be the analogous flow-out in $T^*\mathbb{R}^{n+1}$, so χ takes S_ξ to S_v.

The functions $\theta(z,\xi),\ \rho(z,\xi)$, solving (1.7), with $z = (t,x),\ \eta = \xi_n$, are obtained as follows. Pick $\Phi \in C^\infty(S_v)$ such that $d\Phi = i^*\alpha$, where α is the canonical 1-form on $T^*\Omega$ and $i : S_v \to T^*\Omega$ is the natural inclusion. Φ is determined up to a term independent of z, so normalize it, e.g., by picking a point $q(\xi) \in S_v$ in some smooth convenient fashion and requiring Φ to vanish there. The convexity hypothesis implies that the natural projection

$$\pi : S_v \longrightarrow \Omega \tag{1.16}$$

is a simple fold. One has a smooth involution $j : S_v \to S_v$, interchanging points with the same image under π. With respect to this involution, we will break up Φ into even and odd parts. Let $\Psi = \Phi \circ j$. If S_v is regarded as the graph of the field $v^\pm$, over its image $\pi(S_v)$, define

$$\theta = \frac{1}{2}(\Phi + \Psi) \circ v^\pm, \quad \rho = \xi_1^{1/3}\Big[\frac{3}{4}(\Phi - \Psi) \circ v^\pm\Big]^{2/3}. \tag{1.17}$$

It is straightforward to verify that $\phi^\pm = \theta \pm (2/3)\xi_1^{-1/2}\rho^{3/2}$ satisfies the eikonal equation $(\phi_t^\pm)^2 = (\nabla_x \phi^\pm)^2$ on $\pi(S_v)$, and (1.7) follows. The point of the construction (1.17) is that ρ and θ are smooth up to the image under π of the fold set, the “caustic.” Consequently they can be continued across in a smooth fashion. If $\eta = \xi_n \geq 0,\ S_v$ projects onto a region containing $\partial\Omega$; if $\eta < 0$, this is no longer the case. Thus ρ, θ are defined on Ω for $\eta \geq 0$ by (1.17). Using a formal power series expansion and the Whitney extension theorem, we can smoothly extend ρ, θ to $\eta < 0$ so that the eikonal equation (1.7) is solved to infinite order at the boundary $\partial\Omega$. This is enough to make distributions defined by (1.5) solve the wave equation, mod C^∞, granted an analogous formal solution to the transport equation.

Now we want to look into the behavior of ρ, and verify (1.8). Note that $\rho = 0$ on the caustic set; in particular, on $\partial\Omega$, $\rho = 0$ at $\eta = 0$. Also, we can see that ρ is independent of x on $\partial\Omega$, by studying the eikonal equations, which give

$$v = i^*\Big(d\theta \pm \sqrt{\frac{-\rho}{\xi_1}}\, d\rho\Big) \quad \text{on} \quad \partial\Omega \tag{1.18}$$

(where $i : \partial\Omega \to \Omega$), since v is invariant under the billiard ball maps. This implies $i^* d\rho = 0$, so $\rho|_{\partial\Omega}$ depends on (ξ, η). To see that actually $\rho_{\partial\Omega} = -\eta$, we make use of the fact that ρ, unlike θ, is defined *independently* of the choice of normalization of Φ. Now define $\Phi_0 \in C^\infty(S_\xi)$ in the same fashion as Φ in $C^\infty(S_v)$. If we normalize Φ_0 to vanish at $q_0(\xi) = \chi_J^{-1} q(\xi)$, where Φ was normalized to vanish on $q(\xi)$, then Φ_0 may give rise to a non-smooth θ_0, but we are only concerned with the value of ρ_0, so we proceed. We see that

$$\Phi_0 = \Phi \circ \chi_J. \tag{1.19}$$

Now we know that $(4/3)\rho^{3/2}|_{\partial\Omega}$ is the difference between the two values of $\xi_1^{1/2}\Phi$ at two points in S_v lying over a common image point in $\partial\Omega$. To say these points are so related is equivalent to saying that they both lie in $J_1 \cap K_1$ and are equivalent under the relation $\sim$ defined above. Similarly $(4/3)\rho_0^{3/2}|_{\partial\mathbb{R}^{n+1}_+}$ is the difference between two values of $\xi_1^{1/2}\Phi_0$ at points lying over a common base point in $\partial\mathbb{R}^{n+1}_+$, which is to say these two points are in $J_0 \cap K_0$ and related by $\sim$. Thus χ_J *preserves* this pairing, so

$$\rho\Big|_{\partial\Omega} = \rho_0\Big|_{\partial\mathbb{R}^{n+1}_+}. \tag{1.20}$$

However, in the canonical example, one explicitly has

$$\rho_0 = -\xi_n + x_{n+1}\xi_1, \tag{1.21}$$

and in particular $\rho_0 = -\xi_n = -\eta$ on $\partial\mathbb{R}^{n+1}_+$. This establishes (1.8).

In the constructuon described above, that of θ is not canonical. One can arrange that $\theta|_{\partial\Omega}$ generate the canonical transformation χ_J. In general, whatever canonical transformation it generates has in common with χ_J that it conjugates $\delta^\pm$ to $\delta_0^\pm$.

A parallel but simpler argument produces the amplitudes from certain transport equations, to be solved exactly on Ω for $\eta \geq 0$ and to infinite order for $\eta < 0$, with (1.10) holding.

This sketches the construction of the parametrix (1.5). For more details, and the study of the singularities of (1.5), see the monograph [MeT2], or the earlier exposition in Chapter 10 of [T4], or the original papers [Mel1], [Mel2], [T1]. Of course, the basic result on the singularities of (1.5) is that they lie over $\mathrm{WF}(JF)$ and propagate forward in time along null bicharacteristics of $\partial^2/\partial t^2 - \Delta$, thus verifying the geometrical optics description in the diffractive case.

2. The Neumann operator

The exact solution to the boundary value problem (1.1)–(1.3) can be written as Kirchhoff's integral

$$u(t,x) = \int\limits_{\mathbb{R}\times\partial K} \Big[f(s,y)\frac{\partial G}{\partial\nu}(t-s,x-y) - g(s,y)G(t-s,x-y)\Big]\,ds\,dS(y), \tag{2.1}$$

where

$$g = \frac{\partial u}{\partial\nu}\Big|_{\mathbb{R}\times\partial K} = Nf \tag{2.2}$$

defines the Neumann operator (also called the Dirichlet-to-Neumann map). Here, $G(t,x)$ is the free space fundamental solution to the wave equation on $\mathbb{R}\times\mathbb{R}^n$. For $n=3$, for example, one has

$$G(t,x)=\frac{\delta(|x|-t)}{4\pi t},$$

for $t>0$. Evidently, it is very useful to analyze the properties of N. When K is convex, so the diffractive hypothesis is satisfied, we can analyze N as a pseudodifferential operator, using the parametrix (1.5), as follows.

Differentiate (1.5) and restrict to $\mathbb{R}\times\partial K$. Use (1.8) and (1.10). Note that (1.8) implies $\nabla\rho$ is normal to ∂K, so, if one takes ρ independent of t, which can be arranged, the second half of (1.7) implies $\theta_\nu|_{\partial K}=0$. Thus (1.5) gives

$$\begin{aligned}\frac{\partial u}{\partial\nu}\Big|_{\mathbb{R}\times\partial K}&=\iint(g\rho_\nu+ih_\nu)\xi_1^{-1/3}\frac{A'}{A}(-\xi_1^{-1/3}\eta)\hat{F}(\xi,\eta)e^{i\theta_0}\,d\xi\,d\eta\\&\qquad+\iint g_\nu\hat{F}(\xi,\eta)e^{i\theta_0}\,d\xi\,d\eta\\&=K_1QF+K_2F,\end{aligned}\tag{2.3}$$

where

$$(QF)\hat{}(\xi,\eta)=\xi_1^{-1/3}\frac{A'}{A}(-\xi_1^{-1/3}\eta)\hat{F}(\xi,\eta)\tag{2.4}$$

defines $Q\in OPS^0_{1/3,0}$. The operators K_1 and K_2 are Fourier integral operators with the same phase functions as J; K_1 is elliptic of order 1, and K_2 has order 0. Egorov's theorem gives $K_1=JA,\ K_2=JB$, for certain $A\in OPS^1$ elliptic (not to be confused with the Airy function!), $B\in OPS^0$. Comparing with (1.11), we get

$$N=J(AQ+B)J^{-1}.\tag{2.5}$$

Thus N is conjugated to the special form $AQ+B$, by a Fourier integral operator whose associated canonical transformation is the very one χ_J given in (1.15). The fact that this transformation conjugates the billiard ball maps $\delta^\pm$ to standard form has deep connections with the form of the argument of the airy quotient A'/A in (2.4), as we will see.

Now, look at the conjugate under J of another Fourier multiplier, $\mathcal{A}i$, defined by

$$(\mathcal{A}i\,F)\hat{}(\xi,\eta)=Ai(-\xi_1^{-1/3}\eta)\hat{F}(\xi,\eta).\tag{2.6}$$

We will see more of this in later sections, as an example of a Fourier integral operator with folding canonical relation. For the moment, just think of it as a Fourier integral operator defined in the conic region $\eta>0$, via the expansion

$$Ai(s)=F(s)\,\sin\chi(s),\tag{2.7}$$

where $F(s)$ and $\chi(s)$ are as in (1.6). Thus, in $\{\eta > 0\}$, $\mathcal{A}i$ is a sum of two Fourier integral operators, whose canonical transformations are (with $\eta = \xi_n,\ \xi = (\xi_1, \dots, \xi_n)$)

$$\mathfrak{A}^{\pm}(x,\xi) = \Bigl(x_1 \pm \frac{1}{3}\Bigl(\frac{\xi_n}{\xi_1}\Bigr)^{3/2}, x_2, \dots, x_{n-1}, x_n \pm \Bigl(\frac{\xi_n}{\xi_1}\Bigr)^{1/2}, \xi\Bigr). \tag{2.8}$$

Compare with the "standard" billiard ball map:

$$\delta_0^{\pm}(x,\xi) = \Bigl(x_1 \pm \frac{2}{3}\Bigl(\frac{\xi_n}{\xi_1}\Bigr)^{3/2}, x_2, \dots, x_{n-1}, x_n \pm 2\Bigl(\frac{\xi_n}{\xi_1}\Bigr)^{1/2}, \xi\Bigr). \tag{2.9}$$

Clearly

$$(\mathfrak{A}^{\pm})^2 = \delta_0^{\pm}. \tag{2.10}$$

This gives the following result. The operator $J(\mathcal{A}i^2)J^{-1}$ is an operator which, when restricted to the "hyperbolic" region, is a sum of three Fourier integral operators, whose three canonical relations are the two billiard ball maps, δ^+ and δ^-, and the identity.

Another geometrical phenomenon, emphasized by Melrose [Mel4], involving the canonical transformation χ_J versus the argument $\zeta_0 = \xi_1^{-1/3}\eta$, is the following. Define ζ by $\zeta_0 = \zeta \circ \chi_J$. Consider the Hamiltonian vector field $H_{\zeta^{3/2}}$ and consider its time one flow, Exp $H_{\zeta^{3/2}}$. This is the map δ^+.

As a further remark, we note that the Neumann boundary problem (1.1), (1.3), and (1.4), can be solved using

$$N^{-1} = JQ^{-1}(A + BQ^{-1})^{-1}J^{-1}, \tag{2.11}$$

since $Q^{-1} \in OPS^{1/3}_{1/3,0}$ and $A + BQ^{-1} \in OPS^{1}_{1/3,0}$ is elliptic. A study of the Neumann operator is useful in considering other boundary value problems for the wave equation, including the problem of diffraction of electromagnetic waves by a convex perfect conductor. Details are given in Chapter 10 of [T4].

More material on operators of the form (2.5) and (2.11) can be found in [T7] and in Chapter 9 of [MeT2].

3. Fourier integral operators with folding canonical relations

The operation of convolution by $\delta(x_1 - x_n^3/3)\delta(x_2)\cdots\delta(x_{n-1})$ is a Fourier integral operator with folding canonical relation, i.e., its canonical relation $\Lambda' \subset T^*\mathbb{R}^n \times T^*\mathbb{R}^n$ projects onto each factor as a simple fold. This operation is the same as Fourier multiplication by $\xi_1^{-1/3}Ai(-\xi_1^{-1/3}\xi_n)$. Thus the operator $\mathcal{A}i$ defined by

(2.6) is a Fourier integral operator with folding canonical relation. So is the operator $\mathcal{A}i'$, defined by

$$(\mathcal{A}i'\,F)\widehat{\ }(\xi,\eta)=Ai'(-\xi_1^{-1/3}\eta)\hat{F}(\xi,\eta). \tag{3.1}$$

This is (essentially) convolution by the above distribution, multiplied by x_n. One of the aims of this section is to show that, if $\dim X_1=\dim X_2=n$ and $\Lambda\subset T^*X_1\times T^*X_2$ is a folding canonical relation, then any Fourier integral operator $A\in I^m(X_1,X_2;\Lambda')$ can be written in the form

$$A=J(P_1\mathcal{A}i+P_2\mathcal{A}i')K, \tag{3.2}$$

for some elliptic Fourier integral operators J and K (of order 0) and some

$$P_1\in OPS^{m+1/6},\quad P_2\in OPS^{m-1/6}.$$

We also want to understand the behavior of A^*A.

Suppose $\Lambda'\subset T^*X_1\times T^*X_2$ is a folding canonical relation. We give a condition that guarantees that two elements $A_1,A_2\in I^m(X_1,X_2;\Lambda')$ generate them all, as a module over OPS^0, at least locally near a point on the image of the fold set $L\subset\Lambda'$, projected onto X_1. First we introduce some geometry. The projection π_j of Λ' to T^*X_j determines an involution, which we denote $\mathcal{J}_j$, such that

$$\mathcal{J}_j(\zeta)=\zeta'\ \text{ if }\ \pi_j(\zeta)=\pi_j(\zeta'). \tag{3.3}$$

Note that, for any $P\in OPS^0$, PA has principal symbol which is a multiple p of that of A_1, and $\mathcal{J}_2^*p=p$ on Λ'. This explains why *two* operators are needed to generate $I^m(X_1,X_s;\Lambda')$. Indeed, we have the following.

Proposition 3.1. *Let $\zeta\in L$ (the fold set in Λ'), and suppose $\sigma_{A_1}\neq 0$ at ζ. Let $\sigma_{A_2}=\beta\sigma_{A_1}$ and suppose $\beta-\mathcal{J}_2^*\beta$ vanishes to precisely first order on L, near ζ. Then, microlocally near $\pi_1\zeta$, for any $A\in I^\nu(X_1,X_2;\Lambda')$, you can write, modulo a smoothing operator,*

$$A=P_1A_1+P_2A_2,\quad P_j\in OPS^{\nu-m}. \tag{3.4}$$

Here σ_{A_j} denotes the principal symbol of A_j, a section of the Keller-Maslov line bundle over Λ', and β is scalar.

Proof. The hypothesis implies that any homogeneous (scalar) function g on Λ' can (near ζ) be written in the form

$$g=g_1+g_2\beta,$$

where g_1 and g_2 are homogeneous of the appropriate degree and even with respect to $\mathcal{J}_2$; hence $g_j=\pi_2^*p_j$. Letting P_j have principal symbol p_j, if $\sigma_A=g\sigma_{A_1}$, we get (3.4), modulo $I^{\nu-1}(X_1,X_2;\Lambda')$. An inductive argument finishes the proof.

It is easy to see that the operators $\mathcal{A}i$, $\mathcal{A}i'$ satisfy the hypotheses of Proposition 3.1, after normalization of their order.

The next thing we want to do is show that, given a folding canonical relation $\Lambda' \subset T^*X_1 \times T^*X_2$ ($\dim X_j = n$), there exist homogeneous canonical transformations

$$\chi_j : T^*\mathbb{R}^n \longrightarrow T^*X_j$$

such that

$$\chi_2^{-1} \circ \Lambda' \circ \chi_1 \subset T^*\mathbb{R}^n \times T^*\mathbb{R}^n$$

is the "standard" folding canonical relation associated to $\mathcal{A}i$:

$$C_0(x,\xi) = \Big(x_1 \pm \frac{1}{3}\Big(\frac{\xi_n}{\xi_1}\Big)^{3/2}, x_2, \dots, x_{n-1}, x_n \pm \Big(\frac{\xi_n}{\xi_1}\Big)^{1/2}, \xi\Big). \tag{3.5}$$

First we introduce some geometric objects associated with Λ', in addition to the involutions $\mathcal{J}_j$ discussed above. We also have "boundary maps"

$$\delta_1^{\pm} = \pi_1 \circ \mathcal{J}_2 \circ \pi_1^{-1}, \quad \delta_2^{\pm} = \pi_2 \circ \mathcal{J}_1 \circ \pi_2^{-1}, \tag{3.6}$$

where $\pm$ depends on the choice of continuous inverse of π_1 or π_2. The domain and range of $\delta_j^{\pm}$ is the image under π_j of Λ' in T^*X_j. These boundary maps have the same properties as the billiard ball maps discussed in §1. Indeed, in applications we will see later, $X_1 = \mathbb{R} \times \partial K$ and $\delta_1^{\pm}$ will be the billiard ball map. Furthermore, in the special case when $\Lambda' = C_0$, $\delta_1^{\pm} = \delta_2^{\pm} = \delta_0^{\pm}$, the billiard ball map for the canonical example discussed in §1. There is a simple formula for $\delta_0^{\pm}$:

$$\delta_0^{\pm}(x,\xi) = \Big(x_1 \pm \frac{2}{3}\Big(\frac{\xi_n}{\xi_1}\Big)^{3/2}, x_2, \dots, x_{n-1}, x_n \pm 2\Big(\frac{\xi_n}{\xi_1}\Big)^{1/2}, \xi\Big). \tag{3.7}$$

In §1 we showed that, if $X_1 = \mathbb{R} \times \partial K$ and $\delta_1^{\pm}$ is the billiard ball map, there is a canonical transformation $\chi_1 = \chi_J$ which conjugates $\delta_1^{\pm}$ to $\delta_0^{\pm}$. This holds generally. In fact, Proposition 7.14 of [Mel2] says there exist homogeneous symplectic coordinates (x,ξ) on T^*X_1 with $\xi_n \geq 0$ on $\pi_1(\Lambda')$, such that in these coordinates $\delta_1^{\pm}$ takes the form (3.7). We are now ready to state the main geometrical result.

Proposition 3.2. *If $\Lambda' \subset T^*X_1 \times T^*X_2$ is a folding canonical relation, and if $\chi_1 : T^*\mathbb{R}^n \to T^*X_1$ conjugates $\delta_1^{\pm}$ to $\delta_0^{\pm}$, then there exists a canonical transformation $\chi_2 : T^*\mathbb{R}^n \to T^*X_2$ such that*

$$\chi_2^{-1} \circ \Lambda' \circ \chi_1 = C_0. \tag{3.8}$$

Proof. Replacing Λ' by $\Lambda' \circ \chi_1$, we can suppose $\delta_1^{\pm} = \delta_0^{\pm}$. We look for χ_2 such that $\chi_2 \circ \Lambda' = C_0$. First note that there exist natural maps

$$\chi^{\pm} : \Lambda' \longrightarrow C_0, \tag{3.9}$$

defined as follows. For $p \in \pi_1(\Lambda') = \pi_1(C_0) \subset T^*(\mathbb{R}^n)$, there are two points $q_1(p), q_2(p) \in \Lambda'$ and two points $r_1(p), r_2(p) \in C_0$ mapped to p by π_1, these two points degenerating to one for $p \in \{\xi_n = 0\}$, the image of the fold sets. We can suppose that $q_1(p)$ (resp., $r_1(p)$) belongs to one selected component of the complement of the fold set in Λ' (resp., in C_0), and that $q_2(p)$ (resp. $r_2(p)$) belongs to the other. Then $\chi^{\pm}$ is defined by $\chi^+(q_j(p)) = r_j(p)$, and $\chi^-(q_j(p)) = r_{j'}(p)$, where $1' = 2,\ 2' = 1$. It is not hard to see that $\chi^{\pm}$ are C^∞ and preserve the "folded symplectic forms" on Λ' and C_0, which are the pull backs by π_1^* of the symplectic form on $T^*(\mathbb{R}^n)$. Note that, since $\chi^{\pm}$ each conjugate $\delta_1^{\pm}$ to $\delta_0^{\pm}$, these maps take the involution $\mathcal{J}_2$ on Λ' to the analogous involution $\mathcal{J}_2$ on C_0.

We are ready to define χ_2. First we define χ_2^{-1} on the image $\pi_2(\Lambda')$ in T^*X_2, as follows. Let $p \in \pi_2(\Lambda') \subset T^*X_2$. Let $\pi_2(p_1) = \pi_2(p_2) = p,\ p_j \in \Lambda'$, let $\tilde{p}_j = \chi^+(p_j)$. we claim that

$$\pi_2(\tilde{p}_1) = \pi_2(\tilde{p}_2) \in T^*(\mathbb{R}^n). \tag{3.10}$$

Indeed, (3.10) holds if and only if $\mathcal{J}_2$ interchanges $\tilde{p}_1$ and $\tilde{p}_2$. But by the same token $\mathcal{J}_2$ does interchange p_1 and p_2, and since χ^+ conjugates one $\mathcal{J}_2$ to the other, we have (3.10). So set

$$\chi_2^{-1}(p) = \pi_2(\tilde{p}_1) = \pi_2(\tilde{p}_2). \tag{3.11}$$

From he structure of π_2 as a fold, it follows from (3.11) that χ_2^{-1} is C^∞ on the region with boundary $\pi_1(\Lambda')$. Hence there exists a smooth extension to a neighborhood of the boundary. Pick any one, to define χ_2^{-1}. This completes the proof.

Propositions 3.1 and 3.2 together easily give the following main result.

Theorem 3.3. *If $A \in I^m(X_1, X_2; \Lambda')$ with Λ' a folding canonical relation, then there exist elliptic Fourier integral operators J and K, corrseponding to the canonical transformations χ_2 and χ_1 of Proposition 3.2, such that*

$$A = J(P_1 \mathcal{A}i + P_2 \mathcal{A}i')K, \tag{3.12}$$

for some $P_1 \in OPS^{m+1/6},\ P_2 \in OPS^{m-1/6}$. Furthermore one can fix the canonical transformation associated with K (alternatively, with J) to be any one which conjugates the appropriate boundary maps to the standard form $\delta_0^{\pm}$.

One simple corollary to Theorem 3.3 gives the sharp order of continuity of these FIOs on Sobolev spaces.

Corollary 3.4. *If $A \in I^m(X_1, X_2; \Lambda')$ as in Theorem 3.3, then*

$$A : H^s(X_1) \longrightarrow H^{s-m-1/6}(X_2),$$

for all $s \in \mathbb{R}$. Furthermore, $A : H^s(X_1) \to H^{s-m}(X_2)$, if and only if $\sigma_A|_L = 0$, where $L \subset \Lambda'$ is the fold set.

Proof. This follows from the representation (3.12) by standard continuity results for the FIOs J and K, the pseudodifferential operators P_1 and P_2, and the Fourier multipliers $\mathcal{A}i$ and $\mathcal{A}i'$.

Finally, we analyze A^*PA, given $P \in OPS^{\mu}$. By Theorem 3.3, we have

$$A^*PA = K^*(\mathcal{A}iP_1^* + \mathcal{A}i'P_2^*)J^*PJ(P_1\mathcal{A}i + P_2\mathcal{A}i')K,$$

with $P_1, P_1^* \in OPS^{m+1/6}$, $P_2P_2^* \in OPS^{m-1/6}$. By Egorov's theorem, $J^*PJ \in OPS^{\mu}$. By Proposition 3.1, all the pseudodifferential operators can be pushed to the left of $\mathcal{A}i$ and $\mathcal{A}i'$, and we get

$$A^*PA = K^*(P_{11}\mathcal{A}i^2 + P_{12}\mathcal{A}i\mathcal{A}i' + P_{22}(\mathcal{A}i)^2)K, \tag{3.13}$$

with

$$P_{11} \in OPS^{\mu+2m+1/3}, \quad P_{12} \in OPS^{\mu+2m}, \quad P_{22} \in OPS^{\mu+2m-1/3}. \tag{3.14}$$

This puts A^*PA in a standard form. Note that

$$\mathrm{WF}(A^*PAu) \subset \mathcal{C} \circ \mathrm{WF}(u), \tag{3.15}$$

where the "canonical relation" $\mathcal{C}$ is the union of two Lagrangian manifolds:

$$\mathcal{C} = \widetilde{\Lambda} \cup \Delta^+. \tag{3.16}$$

$\widetilde{\Lambda}$ is a folding canonical relation and Δ^+ is a Lagrangian manifold with boundary (a subset of the diagonal) transversally intersecting $\widetilde{\Lambda}$, the intersection coinciding with the fold set for $\widetilde{\Lambda}$.

4. The scattering operator

The scattering operator gives information on the behavior at infinity of solutions to the wave equation. It is related to the scattering amplitude $a_s(\theta, \omega, \lambda)$, which gives the large x behavior of the "outgoing" solution to the boundary value problem for $u_s = u_s(\lambda, x, \omega)$:

$$(\Delta + \lambda^2)u_s = 0 \ \text{ on } \ \mathbb{R}^3 \setminus K, \quad u_s\Big|_{\partial K} = e^{-i\lambda x\cdot\omega}, \tag{4.1}$$

namely

$$a_s(\theta, \omega, \lambda) = \lim_{r\to\infty} re^{-i\lambda r}u_s(\lambda, r\theta, \omega). \tag{4.2}$$

The scattering operator is the operator with kernel $\hat{a}_s(\theta,\omega,s-t)$, where

$$\hat{a}_s(\theta,\omega,t) = \int_{-\infty}^{\infty} a_s(\theta,\omega,\lambda)e^{-i\lambda t}\,d\lambda. \tag{4.3}$$

Since the outgoing solution to (4.1) can be written

$$u_s(x) = \int\limits_{\partial K} \Big[u_s(y)\frac{\partial G_\lambda}{\partial\nu}(x-y) - \frac{\partial u_s}{\partial\nu}G_\lambda(x-y)\Big]\,dS(y), \tag{4.4}$$

where $G_\lambda(x) = e^{i\lambda|x|}/|x|$, applying (4.2) gives

$$a_s(\theta,\omega,\lambda) = \int\limits_{\partial K} e^{-i\lambda\theta\cdot y}\Big[i\lambda(\nu\cdot\theta)u_s(\lambda,y,\omega) + \frac{\partial}{\partial\nu}u_s(\lambda,y,\omega)\Big]\,dS(y). \tag{4.5}$$

From (4.3) we get a formula for the kernel of the scattering operator:

$$\hat{a}_s(\theta,\omega,t) = \int\limits_{\partial K} \Big(\frac{\partial}{\partial\nu} - (\nu\cdot\theta)\frac{\partial}{\partial t}\Big)w(t+y\cdot\theta,y,\omega)\,dS(y), \tag{4.6}$$

where w solves the boundary value problem

$$\Big(\frac{\partial^2}{\partial t^2} - \Delta\Big)w = 0, \quad w\Big|_{\mathbb{R}\times\partial K} = \delta(t-y\cdot\omega), \quad w = 0 \ \text{ for } \ t << 0.$$

We can write (4.6) as

$$S = T(N+P)U, \tag{4.7}$$

where N is the Neumann operator of §2, $P = -(\nu\cdot\theta)\partial_t \in OPS^1$, and the operators T and U are defined as follows. $T : \mathcal{E}'(\mathbb{R}\times\partial K) \to \mathcal{E}'(\mathbb{R}\times S^2)$ is given by

$$TF(t,\theta) = \int\limits_{\partial K} F(t+y\cdot\theta,y)\,dS(y), \tag{4.8}$$

and $U : \mathcal{E}'(\mathbb{R}\times S^2) \to \mathcal{E}'(\mathbb{R}\times\partial K)$ is given by

$$Uf(t,y) = \int\limits_{S^2} f(t-y\cdot\omega,\omega)\,d\omega. \tag{4.9}$$

We first point out some basic geometric properties of the operators T and U, so that the results of §3 will be seen to apply. We assume $K\subset\mathbb{R}^3$ is convex, with smooth boundary and strictly positive curvature.

Proposition 4.1. *T and U are Fourier integral operators of order -1 with folding canonical relations, which are inverses of each other. The boundary maps $\delta^{\pm}$ on $T^*(\mathbb{R}\times\partial K)$ are the billiard ball maps.*

Proof. Direct consequence of the formulas (4.8) and (4.9).

Consequently, we have

$$\begin{aligned} U &= J(P_1\mathcal{A}i + P_2\mathcal{A}i')K, \\ T &= K^{-1}(\tilde{P}_1\mathcal{A}i + \tilde{P}_2\mathcal{A}i')J^{-1}, \end{aligned}$$

for certain $P_1, \tilde{P}_1 \in OPS^{-1+1/6}$ and $P_2, \tilde{P}_2 \in OPS^{-1-1/6}$. Here J is the same elliptic FIO that puts the Neumann operator in standard form; see (2.5). Thus (4.7) yields

$$S = K^{-1}(\tilde{P}_1\mathcal{A}i + \tilde{P}_2\mathcal{A}i')(AQ + B + J^{-1}PJ)(P_1\mathcal{A}i + P_2\mathcal{A}i')K. \tag{4.11}$$

Collapsing terms gives

$$S = K^{-1}(P_{00}\mathcal{A}i^2 + P_{01}\mathcal{A}i\mathcal{A}i' + P_{11}(\mathcal{A}i')^2)K, \tag{4.12}$$

where $P_{00} \in OP\mathcal{N}^{-1+1/3}_{1/3}$ has the form

$$P_{00} = P^c_{00} + \sum_{\alpha\geq 0} P_{00\alpha}Q^{(\alpha)}, \tag{4.13}$$

with $P^c_{00}, P_{00\alpha} \in OPS^{-1+1/3}$, $Q^{(\alpha)}$ having symbol $D^{\alpha}_{\xi,\eta}\sigma_Q$, and similarly $P_{01} \in OP\mathcal{N}^{-1}_{1/3}$, $P_{11} \in OP\mathcal{N}^{-1-1/3}_{1/3}$, with asymptotic expansions similar to (4.13).

We next investigate the fact that the wave front relation of S is smaller than that of general operators whose form is given by the right side of (4.12). Indeed, in the shadow region one has $(N + (\nu\cdot\omega)\partial_t)\delta(t - y\cdot\omega) \in C^\infty$. Meanwhile, Green's theorem implies

$$\int_{\partial K} \nu\cdot(\omega+\theta)\delta'(t - x\cdot(\omega-\theta))\,dS(x) = 0,$$

so

$$S\delta_{(0,\omega)} = T\Big(N + (\nu\cdot\omega)\frac{\partial}{\partial t}\Big)\delta(t - y\cdot\omega).$$

Thus $S\delta_{(0,\omega)}$ is singular at $t = \min_{y\in\partial K} y\cdot(\theta-\omega)$, but the singularity at $t = \max_{y\in\partial K} y\cdot(\theta-\omega)$, which would occur for most distributions of the form (4.12), is absent.

In fact, we can get an alternative formula for $S = T(N+P)U$ whose form more closely reflects this restriction on the wave front relation of S, as follows. We have

$$S\delta_{(0,\omega)} = T(N + (\nu\cdot\omega)\partial_t)U\delta_{(0,\omega)}, \tag{4.14}$$

and, for certain $P_1^{\#} \in OPS^{-1+1/6}$, $P_2^{\#} \in OPS^{-1-1/6}$, we have

$$A^{-1}J^{-1}(N+(\nu\cdot\omega)\partial_t)UK^{-1} = Q(P_1\mathcal{A}i + P_2\mathcal{A}i') + P_1^{\#}\mathcal{A}i + P_2^{\#}\mathcal{A}i'. \tag{4.15}$$

Rewrite the right side of (4.15) as

$$Q(\mathcal{A}i\tilde{P}_1 + \mathcal{A}i'\tilde{P}_2) + \mathcal{A}i\tilde{P}_3 + \mathcal{A}i'\tilde{P}_4. \tag{4.16}$$

Using the Wronskian relation

$$Ai' = \frac{\alpha}{A_-} + \frac{A_-'}{A_-}Ai, \quad \alpha \neq 0,$$

write (4.16) as

$$\mathcal{A}i(Q^2\hat{P}_2 + Q(\tilde{P}_1 + \hat{P}_4) + P_3) + \alpha\mathcal{A}_-^{-1}(Q\tilde{P}_2 + \tilde{P}_4). \tag{4.17}$$

We now use the following result.

Lemma 4.2. *Suppose $A, B, C \in OPS^0$ and*

$$V = AQ^2 + BQ + C \in OPS^{-\infty} \quad \textit{on} \quad \{\eta > 0\}. \tag{4.18}$$

Then the terms in the asymptotic expansion of the symbols of A, B, and C all vanish to infinite order at $\eta = 0$ and

$$(AQ^2 + BQ + C)\mathcal{A}i \in OPS^{-\infty}. \tag{4.19}$$

Proof. Note that the symbols of Q and Q^2 have, respectively, the asymptotic expansions

$$\begin{aligned} q &\sim \xi_1^{-1/3}\Big(\beta_0(\xi_1^{-1/3}\eta)^{1/2} + \beta_1(\xi_1^{-1/3}\eta)^{-1} + \beta_2(\xi_1^{-1/3}\eta)^{-5/2} + \cdots\Big), \\ q^2 &\sim \xi_1^{-2/3}\Big(\gamma_0\xi_1^{-1/3}\eta + \gamma_1(\xi_1^{-1/3}\eta)^{-1/2} + \gamma_2(\xi_1^{-1/3}\eta)^{-2} + \cdots\Big). \end{aligned}$$

Let the symbol of A be asymptotic to $\sum A_j$, etc. Then the part homogeneous of degree $-j$ in the expansion of V in $\eta > 0$ is

$$\begin{aligned} V_j = A_j &+ \beta_0\xi_1^{-1/2}\eta^{1/2}B_j + \gamma_0\xi_1^{-1}\eta C_j \\ &+ \beta_1\eta^{-1}B_{j-1} + \gamma_1\xi_1^{-1/2}\eta^{-1/2}C_{j-1} \\ &+ \cdots \\ &+ \beta_j\xi_1^{-1/2+j/2}\eta^{1/2-3j/2}B_0 + \gamma_j\xi_1^{-1+j/2}\eta^{1-3j/2}C_0 \\ = 0.& \end{aligned}$$

Separating terms into integer or non-integer powers of η, we get a pair of equations holding to infinite order at $\eta = 0$, for each j. For each k, we get $2j$ equations in $3k$ unknowns $\eta^\ell A_\ell, \eta^\ell B_\ell, \eta^\ell C_\ell$, mod $O(\eta^k)$ $(0 \le \ell \le k-1)$ and if j is picked so $j > k$, one has uniqueness: $\eta^\ell A_\ell = \eta^\ell B_\ell = \eta^\ell C_\ell = 0$ mod $O(\eta^k)$, $0 \le \ell < k$. Taking k arbitrarily large gives A_j, B_j, C_j all vanishing to infinite order at $\eta = 0$. From this fact, (4.19) is a simple consequence.

To see how the lemma applies to (4.17), note that the first term must have wave front relation constained in that of $\mathcal{A}_-^{-1}$, and since $\mathcal{A}i$ is a sum of two elliptic FIOs in the open cone $\eta > 0$, this implies that $Q^2\hat{P}_2 + Q(\tilde{P}_1 + \hat{P}_4) + P_3$ belongs to $OPS^{-\infty}$ on $\eta > 0$. Taking adjoints, we can apply the lemma, and taking adjoints back implies

$$\mathcal{A}i(Q^2\hat{P}_2 + Q(\tilde{P}_1 + \hat{P}_4) + P_3) \in OPS^{-\infty}. \tag{4.20}$$

We also have all the terms in the asymptotic expansion of $\hat{P}_2$, and hence of $\tilde{P}_2$, vanishing to infinite order at $\eta = 0$, which gives

$$\alpha(Q\tilde{P}_2 + \tilde{P}_4) = P_5 \in OPS^{-1-1/6}.$$

Thus (4.15) gives

$$(N + (\nu \cdot \omega)\partial_t)U = JA\mathcal{A}_-^{-1}P_5K. \tag{4.21}$$

Consequently, using the representation

$$T = K^{-1}(\tilde{P}_1\mathcal{A}i + \tilde{P}_2\mathcal{A}i')J^{-1},$$

we get

$$S = K^{-1}(\tilde{P}_1\mathcal{A}i + \tilde{P}_2\mathcal{A}i')A\mathcal{A}_-^{-1}P_5K,$$

or

$$S = K^{-1}(P_1^b\mathcal{A}i + P_2^b\mathcal{A}i')\mathcal{A}_-^{-1}P_5K. \tag{4.22}$$

We remark that P_5 is elliptic. This follows from the ellipticity of $\tilde{P}_4$, or of $\hat{P}_4$, which in turn follows from the ellipticity of $\tilde{P}_1$, hence of P_1. Thus one could replace P_5K by K in (4.22) and effectively absorb the P_5 factor. We summarize as follows.

Theorem 4.3. *The scattering operator has the form*

$$S = K^{-1}(P_1^{\#}\mathcal{A}i + P_2^{\#}\mathcal{A}i')\mathcal{A}_-^{-1}K, \tag{4.23}$$

where K is an elliptic FIO of order 0, and

$$P_1^{\#} \in OPS^{-1}, \quad P_2^{\#} \in OPS^{-1-1/3}. \tag{4.24}$$

For further details, and results on the scattering amplitude, we refer to [MeT].

5. The corrected Kirchhoff approximation

As one can see from §4, it is desirable to have a good hold on the normal derivative $\partial u_s/\partial\nu$ of the solution to the boundary value problem

$$(\Delta+\lambda^2)u_s = 0 \ \text{ on } \ \mathbb{R}^3\setminus K, \quad u_s\Big|_{\partial K} = e^{-i\lambda x\cdot\omega}, \tag{5.1}$$

satisfying the outgoing condition

$$u_s(x) = O(|x|^{-1}), \quad \frac{\partial u_s}{\partial r} - i\lambda u_s = o(|x|^{-1}), \tag{5.2}$$

as $|x|\to\infty$. This is a classical problem, and a classical tool used in calculations in non-rigorous scattering theory is the Kirchhoff approximation:

$$\frac{\partial u_s}{\partial \nu}\Big|_{\partial K} \approx i\lambda|\nu\cdot\omega|e^{-i\lambda x\cdot\omega}. \tag{5.3}$$

This approximation was proposed by G. Kirchhoff in [Kir], in an effort to cast light on the Fresnel theory of diffraction. It was motivated by the idea that the scattered field, for large λ, is approximately obtained, at a point $x\in\partial K$ where $\nu\cdot\omega>0$ (the "illuminated region") by replacing ∂K by its tangent plane at x and solving the wave equation exactly, and at a point $x\in\partial K$ where $\nu\cdot\omega<0$ (the "shadow region") by the consideration that the total field should be essentially zero.

Rigorous affirmation of (5.3), for K smooth and strictly convex, with positive curvature, was first given in [T4], where it was shown that, with

$$\frac{\partial u_s}{\partial \nu}\Big|_{\partial K} = K(x,\lambda,\omega)e^{-i\lambda x\cdot\omega}, \tag{5.4}$$

there is the estimate

$$\Big|K(x,\lambda,\omega) - i\lambda|\nu\cdot\omega|\Big| \le C_\varepsilon\lambda^{3/4+\varepsilon},$$

for each $\varepsilon>0$. This estimate made use of L^p estimates for operators in $OP\mathcal{N}^0_\rho$, and pushed techniques developed in [MjT]. An analogous estimate for the validity of the Kirchhoff approximation for the Neumann boundary condition and for the natural boundary problem for Maxwell's equations was given by Yingst [Y].

Here we sketch work in [MeT], yielding a complete asymptotic expansion for the coefficient K in (5.4), giving a corrected form of the Kirchhoff approximation. A byproduct is a sharpening of the estimate (5.5) to

$$\Big|K(x,\lambda,\omega) - i\lambda|\nu\cdot\omega|\Big| \le C\lambda^{2/3}. \tag{5.6}$$

Of course, the most interesting aspect of the result is the analysis of the nature of the transition of the normal derivative of the scattered wave across the shadow boundary.

We apply our study of the Neumann operator. First, a simple calculation gives the formula

$$N\Big(e^{-i\lambda(x\cdot\omega-t)}\Big)=e^{i\lambda t}\,\frac{\partial u_s}{\partial\nu}\Big|_{\partial K}. \tag{5.7}$$

So, with $\psi=x\cdot\omega-t|_{\mathbb{R}\times\partial K}$, we have

$$\frac{\partial u_s}{\partial\nu}=e^{-i\lambda t}N(e^{-i\lambda\psi}). \tag{5.8}$$

We are led to apply the Neumann operator N to the oscillatory term $e^{-i\lambda\psi}$. Because the Neumann operator is not a pseudodifferential operator of classical type, the main technical problem is to figure out how to do this. The first key result, about the geometrical relation between the phase function ψ and the operator J, proved by Melrose in [Mel4], is the following.

Lemma 5.1. *The Neumann operator can be written in the form (2.5) with J so chosen that*

$$J^{-1}(e^{-i\lambda\psi})=a(x,y,\lambda)e^{-i\lambda\tilde{\psi}}, \tag{5.9}$$

where $a\in S^0$ and

$$\tilde{\psi}(x,y)=x_1+\frac{y^3}{3}. \tag{5.10}$$

Here, x represents the variables to which ξ are dual, with η dual to y.

The next step is to examine $(\mathcal{A}'/\mathcal{A})(e^{-i\lambda\tilde{\psi}})$. A calculation gives

$$\frac{\mathcal{A}'}{\mathcal{A}}(e^{-i\lambda\tilde{\psi}})=e^{-i\lambda x_1}\Phi(\lambda^{1/3}y), \tag{5.11}$$

where Φ is given by an integral of Fock type:

$$\Phi(\tau)=\int\frac{A'}{A}(s)\,Ai(s)\,e^{-i\tau s}\,ds=\frac{A'}{A}(D_\tau)(e^{i\tau^3/3}). \tag{5.12}$$

The asymptotic expansion of $\Phi(\tau)$ is given as follows. Set

$$r(s)=\frac{A'}{A}(s). \tag{5.13}$$

We have $r\in S^{1/2}(\mathbb{R})$, i.e.,

$$r(s)\sim\sum_{j\geq 0}r_j^{\pm}s^{1/2-j},\quad \text{as}\quad s\to\pm\infty.$$

Lemma 5.2. $\Phi(\tau) = e^{i\tau^3/3}\Psi(\tau)$ *with* $\Psi \in S^1(\mathbb{R})$. *Indeed, as* $|\tau| \to \infty$,

$$\Psi(\tau) \sim \sum_{k\geq 0} \frac{i^k}{k!} \partial_s^k a(0,\tau) r^{(k)}(\tau^2), \tag{5.14}$$

where

$$a(s,\tau) = e^{-is^3/3 - i\tau s^2}. \tag{5.14A}$$

Proof. We can rewrite the far right side of (5.12) as

$$e^{i\tau^3/3}\, r(D_s)\Big(b(s,\lambda)e^{i\lambda s}\Big)\Big|_{s=0,\lambda=\tau^2}, \tag{5.14B}$$

where

$$b(s,\lambda) = a(s,\lambda^{1/2}) \in S^0_{1/2,1/2}.$$

Mod $O(\lambda^{-\infty})$, all the contribution comes from a small neighborhood of $s = 0$, and the pseudodifferential calculus yields (5.14) from (5.14B).

Note that the term $k = 1$ in (5.14) vanishes, and

$$\Psi(\tau) = \frac{A'}{A}(\tau^2) + \rho(\tau), \quad \rho \in S^{-2}(\mathbb{R}). \tag{5.15}$$

So far, we have

$$\frac{\mathcal{A}'}{\mathcal{A}}(e^{-i\lambda\tilde{\psi}}) = \Psi(\lambda^{1/3}y)e^{-i\lambda\tilde{\psi}}. \tag{5.16}$$

It follows that

$$(AQ+B)(J^{-1}e^{-i\lambda\psi}) = \tilde{b}(x,y,\lambda)e^{-i\lambda\tilde{\psi}}, \tag{5.17}$$

with

$$\tilde{b} \sim \sum_{j,k,\ell\geq 0} \sigma_{jk\ell}(x,y,\lambda)\Psi_{jk}^{(\ell)}(\lambda^{1/3}y) + \sum_{j\geq 0} \tau_j(x,y,\lambda), \tag{5.18}$$

where

$$\sigma_{jk\ell} \in S^{2/3-j/3-k-2\ell/3}, \quad \tau_j \in S^{-j}, \quad \Psi_{jk} \in S^{1-2j}(\mathbb{R}).$$

Here, Ψ_{jk} is defined by

$$\begin{aligned} \Psi_{jk}(\tau) &= e^{-i\tau^3/3} r_{jk}(D_\tau)(e^{i\tau^3/3}) \\ &\sim \sum_{\ell\geq 0} \frac{i^\ell}{\ell!} \partial_s^\ell a(0,\tau) r_{jk}^{(\ell)}(\tau^2), \end{aligned} \tag{5.19}$$

where $a(s,\tau)$ is as in (5.14A) and

$$r_{jk}(\lambda) = \lambda^k r^{(j+k)}(\lambda). \tag{5.20}$$

It remains to apply the Fourier integral operator J to the right side of (5.17). We have $\tilde{b} \in S^1_{2/3,1/3}$. Since $2/3 > 1/2$, classical methods apply to the asymptotic expansion of $J(\tilde{b}e^{-i\lambda\tilde{\psi}})$, and one achieves the following result.

Theorem 5.3. *The corrected Kirchhoff formula is*

$$\frac{\partial u_s}{\partial \nu}\Big|_{\partial K} = K(x,\lambda,\omega)e^{-i\lambda x\cdot\omega}, \tag{5.21}$$

where $K \in S^1_{2/3,1/3}$ *has the expansion*

$$K(x,\lambda,\omega) \sim \sum_{j,k,\ell\geq 0} \kappa_{jk\ell}(x,\lambda,\omega)\Psi^{(\ell)}_{jk}(\lambda^{1/3}Z) + K^c(x,\lambda,\omega), \tag{5.22}$$

with

$$K^c \in S^0, \quad \kappa_{jk\ell} \in S^{2/3-j/3-k-2\ell/3+a(\ell)},$$

where $a(0)=a(1)=0$ *and* $a(\ell)=1$ *for* $\ell \geq 2$*. Furthermore,*

$$Z \text{ vanishes to first order on } \{\nu\cdot\omega = 0\}. \tag{5.23}$$

We record all the terms of order greater than zero. We have

$$\begin{aligned} K = &-\frac{\nu\cdot\omega}{Z}\,\lambda^{2/3}\Big[\frac{A'}{A}(\lambda^{2/3}Z^2) + \rho(\lambda^{1/3}Z)\Big] \\ &+ \kappa_{100}\Psi_{10}(\lambda^{1/3}Z) + \kappa_{002}\Psi^{(2)}_{00}(\lambda^{1/3}Z), \\ &\text{mod } S^0_{2/3,1/3}. \end{aligned} \tag{5.24}$$

Here, ρ is given by (5.15), Ψ_{10} and Ψ_{00} by (5.19), and $\kappa_{100}, \kappa_{002} \in S^{1/3}$. From (5.24) it is apparent that $\lambda^{2/3}$ is the best possible power of λ that could go on the right side in (5.6).

6. A representation for the wave evolution operator

This section discusses some results of Farris [F1], [F2], to which we refer for further details. We want to look at the structure of the solution operator $e^{iT\sqrt{-\Delta}}$ at a fixed time T. Here, Δ is the Laplace operator on $\mathbb{R}^n \setminus K$, with the Dirichlet boundary condition on ∂K. More generally, Δ could be defined on a complete Riemannian manifold M with compact diffractive boundary. Let $\mathcal{O}$ be bounded away from ∂M, and suppose T is picked so that, if we consider all the geodesics issuing from $\overline{\mathcal{O}}$, reflecting off ∂M by the usual rules of geometrical optics, the set U of endpoints of distance T from their origins, avoids ∂M. It follows that, for $u \in \mathcal{E}'(\mathcal{O})$, $e^{iT\sqrt{-\Delta}}u$ is C^∞ near ∂M. The goal here is to show that this operator is of the form (mod C^∞)

$$e^{iT\sqrt{-\Delta}}u = K_2\frac{\mathcal{A}_+}{\mathcal{A}_-}K_1 u, \quad u \in \mathcal{E}'(\mathcal{O}), \tag{6.1}$$

where K_1, K_2 are elliptic FIOs (depending on T) and the operator $\mathcal{A}_+/\mathcal{A}_-$ is Fourier multiplication:

$$\Big(\frac{\mathcal{A}_+}{\mathcal{A}_-}F\Big)\hat{}(\xi,\eta) = \frac{A_+}{A_-}(-\xi_1^{-1/3}\eta)\hat{F}(\xi,\eta). \tag{6.2}$$

To start, let Δ_0 be the free space Laplacian, on $\mathbb{R}^n$, or more generally on some complete, boundaryless manifold $\widetilde{M}$ containing M. Let

$$F = e^{iT\sqrt{-\Delta_0}},$$

and let $R : \mathcal{E}'(\mathcal{O}) \to \mathcal{D}'(\mathbb{R}\times\partial M)$ be given by

$$Ru = e^{it\sqrt{-\Delta_0}}u\Big|_{\mathbb{R}\times\partial M}. \tag{6.3}$$

Also, let $E : \mathcal{E}'(\mathbb{R}\times\partial M) \to \mathcal{D}'(M)$ be defined as follows: Ef is the value at $t = T$ of the outgoing solution w to the wave equation on $\mathbb{R}\times M$ ($w = 0$ for $t << 0$) with boundary condition $w|_{\mathbb{R}\times\partial M} = f$. Then ER is well defined and

$$e^{iT\sqrt{-\Delta}} = F - ER. \tag{6.4}$$

The map E is produced by taking (1.5) (with $F = J^{-1}f$) and evaluating at $t = T$. Note that, if $\mathrm{WF}(F)$ is in a small conic neighborhood of $\eta = 0$, which we may assume without loss of generality, then away from ∂M one can replace $A(\xi_1^{-1/3}\rho)$ and $A'(\xi_1^{-1/3}\rho)$ by their asymptotic expansions, by (1.9), and write

$$E = L\mathcal{A}_-^{-1}J^{-1}, \tag{6.5}$$

where (using a cutoff $\phi(\xi_1^{-1}\eta)$)

$$LF = \int \big[gA_-(\xi_1^{-1/3}\rho) + ih\xi_1^{-1/3}A_-'(\xi_1^{-1/3}\rho)\big]e^{i\theta}\hat{F}\,d\xi\,d\eta, \tag{6.6}$$

the integral being evaluated at $t = T$ and restricted to $x \in U$. L is a classical FIO, and if we restrict our attention to near the boundary ∂M, L is elliptic.

The map R is a Fourier integral operator with folding canonical relation, and the boundary maps $\delta^\pm$ on $T^*(\mathbb{R}\times\partial M)$ are easily seen to coincide with the billiard ball maps. Thus, by §3, one can write

$$J^{-1}RK = \tilde{P}_1\mathcal{A}i + \tilde{P}_2\mathcal{A}i', \tag{6.7}$$

for some pseudodifferential operators $\tilde{P}_j$ and some elliptic Fourier integral operators J and K, and in fact J can be taken to be the operator (1.11), which enters into the formula for the Neumann operator (2.5). Combining (6.5) and (6.7) gives

$$ER = L\mathcal{A}_-^{-1}(\tilde{P}_1\mathcal{A}i + \tilde{P}_2\mathcal{A}i')K^{-1}. \tag{6.8}$$

In fact, we claim that K can be taken to be the operator

$$KF = \int \big[gA_+(\xi_1^{-1/3}\rho) + ihA'_+(\xi_1^{-1/3}\rho)\big] e^{i\theta} \hat{F}\, d\xi\, d\eta, \tag{6.9}$$

the integral evaluated at $t = 0$. Note that

$$E^- = K\mathcal{A}_+^{-1} J^{-1}, \tag{6.10}$$

where $E^- f$ is the value at $t = 0$ of the *incoming* solution $\tilde{w}$ to the wave equation on $\mathbb{R} \times M$ ($\tilde{w} = 0$ for $t >> 0$) with boundary condition $\tilde{w}|_{\mathbb{R}\times\partial M} = f$. A study of the geometry of these operators shows that $J^{-1}RK$ is a FIO whose folding canonical relation is the standard model C_0. One use of this explicit representation of K is to prove the following.

Lemma 6.1. *$L^{-1}FK$ and its inverse $K^{-1}F^{-1}L$ are elliptic pseudodifferential operators on $\{\eta \geq 0\}$.*

Proof. (Recall that we know these operators are elliptic FIOs.) It suffices to prove the assertion for $\{\eta > 0\}$. Use the representation

$$FK = FE^- J\mathcal{A}_+, \quad L = EJ\mathcal{A}_- \ \text{ on } \ \{\eta > 0\}.$$

Each of these is an elliptic FIO in this region, and to see that they move wave front sets in the same fashion, it suffices to note that

$$J\,\frac{\mathcal{A}_-}{\mathcal{A}_+}\,J^{-1} \tag{6.11}$$

has, in $J\{\eta > 0\}$, the canonical transformation equal to the billiard ball map δ^+. This is established by the same argument used to treat $J\mathcal{A}i^2 J^{-1}$ in §2.

Given this lemma, we have, in addition to (6.3),

$$J^{-1}R(F^{-1}L) = P_1\mathcal{A}i + P_2\mathcal{A}i',$$

and hence, as a convenient modification of (6.8), we have

$$ER = L\mathcal{A}_-^{-1}(P_1\mathcal{A}i + P_2\mathcal{A}i')L^{-1}F. \tag{6.12}$$

Returning to (6.4), we see that, acting on $\mathcal{E}'(\mathcal{O})$,

$$e^{iT\sqrt{-\Delta}} = L[I - \mathcal{A}_-^{-1}(P_1\mathcal{A}i + P_2\mathcal{A}i')]L^{-1}F. \tag{6.13}$$

In order to simplify the factor in brackets, let us note that, by virtue of the known propagation of singularities for the operator $e^{iT\sqrt{-\Delta}}$, the factor in brackets must move wave front sets the same way $\mathcal{A}_+/\mathcal{A}_-$ does. Using

$$\mathcal{A}i = -\overline{\omega}\mathcal{A}_- - \omega\mathcal{A}_+, \quad \omega = e^{(2/3)\pi i},$$

one gets

$$\begin{aligned} &I - \mathcal{A}_-^{-1}(P_1\mathcal{A}i + P_2\mathcal{A}i') \\ &= \frac{\mathcal{A}_+}{\mathcal{A}_-}\big[-\omega^2 - \mathcal{A}_+^{-1}((P_1+\omega)\mathcal{A}i + P_2\mathcal{A}i')\big], \end{aligned} \tag{6.14}$$

and using the Wronskian relation

$$A_-'Ai - A_-Ai' = \alpha, \quad \alpha \neq 0,$$

we rewrite the factor in brackets on the right side of (6.14) as

$$-\omega^2 - \alpha\mathcal{A}_+^{-1}P_2\mathcal{A}_-^{-1} - \mathcal{A}_+^{-1}\Big(P_1 + \omega - P_2\frac{\mathcal{A}_-'}{\mathcal{A}_-}\Big)\mathcal{A}i. \tag{6.15}$$

Now this operator, which in the region $\{\eta > 0\}$ is a classical FIO, is supposed to preserve wave front sets. In particular, the last term in (6.15) is supposed to preserve wave front sets. This implies that

$$P_1 + \omega - P_2\frac{\mathcal{A}_-'}{\mathcal{A}_-} \in OPS^{-\infty} \ \text{ on } \ \{\eta > 0\}. \tag{6.16}$$

Since P_1 and P_2 are classical pseudodifferential operators, (6.16) is a very stringent condition. Indeed, one has the following, which is in fact a special case of Lemma 4.2.

Lemma 6.2. *Let $A, B \in OPS^m$. Suppose*

$$A + BQ \in OPS^{-\infty} \quad \textit{on} \quad \{\eta > 0\}. \tag{6.17}$$

Then all the terms in the asymptotic expansions of the symbols of A and B must vanish to infinite order at $\eta = 0$, and

$$(A + BQ)\mathcal{A}_\pm^{-1}, \quad (A + BQ)\mathcal{A}i \in OPS^{-\infty}. \tag{6.18}$$

Proof. Replacing $(A'/A)(-\xi_1^{-1/3}\eta)$ by its asymptotic expansion gives an infinite set of identities, from (6.17), a priori satisfied for $\eta > 0$, hence, by continuity, satisfied for $\eta \geq 0$. For the principal symbols one gets

$$a_0 + b_0\sqrt{\frac{\eta}{\xi_1}} = 0,$$

which implies a_0 and b_0 vanish to infinite order at $\eta = 0$. Such vanishing of higher order terms follows inductively, and from this, (6.18) is an elementary consequence.

Applying the lemma to (6.16), we conclude that the expression (6.15) is equal to

$$-\omega^2 - \alpha\mathcal{A}_+^{-1}P_2\mathcal{A}_-^{-1}, \quad \text{mod } \ OPS^{-\infty}, \tag{6.19}$$

and that

$$P_2 \text{ vanishes to infinite order at } \ \eta = 0. \tag{6.20}$$

From (6.20), one can adapt a proof of Egorov's theorem to get

$$\alpha\mathcal{A}_+^{-1}P_2\mathcal{A}_-^{-1} = P_3 \in OPS^0. \tag{6.21}$$

Putting together (6.13)–(6.15) with (6.19)–(6.21), we have the main result:

Theorem 6.3. *Acting on $\mathcal{E}'(\mathcal{O})$,*

$$e^{iT\sqrt{-\Delta}} = L\frac{\mathcal{A}_+}{\mathcal{A}_-}(-\omega^2 - P_3)L^{-1}e^{iT\sqrt{-\Delta_0}}, \tag{6.22}$$

mod $OPS^{-\infty}$. Here, L is the elliptic FIO arising in (6.6) and $P_3 \in OPS^0$ is given by (6.21).

This representation allows one to analyze

$$e^{iT\sqrt{-\Delta}}\, P\, e^{-iT\sqrt{-\Delta}}, \tag{6.23}$$

given $P \in OPS^m(M)$, with symbol supported in $\mathcal{O}$, as a pseudodifferential operator, of non-classical type, with symbol essentially supported in U. This new operator can be regarded as having a "principal symbol" which is continuous, but not smooth, on the cosphere bundle of M, and then Egorov's theorem holds; the two principal symbols are related by the (non smooth) canonical transformation associated with $e^{iT\sqrt{-\Delta}}$. For details, see [F2].

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