GAUSSIAN BEAM METHODS FOR THE HELMHOLTZ EQUATION[*]

HAILIANG LIU[†], JAMES RALSTON[‡], OLOF RUNBORG[§], AND
NICOLAY M. TANUSHEV[¶]

Abstract. In this work we construct Gaussian beam approximations to solutions of the high frequency Helmholtz equation with a localized source. Under the assumption of nontrapping rays we show error estimates between the exact outgoing solution and Gaussian beams in terms of the wave number k, both for single beams and superposition of beams. The main result is that the relative local L^2 error in the beam approximations decay as $k^{-N/2}$ independent of dimension and presence of caustics for Nth order beams.

Key words. Helmholtz equation, high frequency wave propagation, localized source, radiation condition

AMS subject classifications. 35B45, 35J05, 35Q60, 78A40

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1. Introduction. In this paper, we are interested in the accuracy of Gaussian beam approximations to solutions of the high frequency Helmholtz equation with a source term,

$$(1) \qquad L_n u =_{def} \Delta u + (i\alpha k + k^2)n^2 u = f, \qquad x \in \mathbb{R}^d.$$

Here $k > 0$ is the wave number, assumed to be large, $n(x)$ is the index of refraction, and $f(x; k)$ is a source function, which in general can also depend on k. We assume that both $f(x; k)$ and $n(x) - 1$ vanish for $|x| > R$. The nonnegative parameter α represents absorption. It is zero in the limit of zero absorption, where L^2 solutions of (1) become solutions satisfying the standard radiation condition. We will construct approximations to the radiating solution of (1) in the case when f is supported on a hyperplane and will give precise results on their convergence as $k \to \infty$.

The Helmholtz equation (1) is widely used to model wave propagation problems in application areas such as electromagnetics, geophysics, and acoustics. Numerical simulation of the Helmholtz equation becomes expensive when the frequency of the waves is high. In direct discretization methods, a large number of grid points is needed to resolve the wave oscillations and the computational cost to maintain constant accuracy grows algebraically with the frequency. The Helmholtz equation is typically even more difficult to handle in this regime than time-dependent wave equations, as numerical discretizations lead to large indefinite and ill-conditioned linear systems of equations, for which it is difficult to find efficient preconditioners [11]. At sufficiently high frequencies direct simulations are not feasible.

[†]Department of Mathematics, Iowa State University, Ames, IA 50010 (hliu@iastate.edu).

[‡]Department of Mathematics, University of California at Los Angeles, Los Angeles, CA 90095 (ralston@math.ucla.edu).

[§]Department of Mathematics and Swedish e-Science Research Center (SeRC), KTH, 10044 Stockholm, Sweden (olofr@nada.kth.se).

[¶]Z-Terra Inc., 17171 Park Row, Suite 247, Houston, TX 77084 (nick.tanushev@gmail.com).

As an alternative one can use high frequency asymptotic models for wave propagation, such as geometrical optics [28, 10, 43], which is obtained when the frequency tends to infinity. The solution of the partial differential equation (PDE) is assumed to be of the form

$$(2) \qquad\qquad u = ae^{ik\phi},$$

where ϕ is the phase, and a is the amplitude of the solution. In the limit $k \to \infty$ the phase and amplitude are independent of the frequency and vary on a much coarser scale than the full wave solution. Therefore, they can be computed at a computational cost independent of the frequency. However, a main drawback of geometrical optics is that the model breaks down at caustics, where rays concentrate and the predicted amplitude a becomes unbounded.

Gaussian beams form another high frequency asymptotic model which is closely related to geometrical optics. However, unlike geometrical optics, the phase ϕ is complex-valued, and there is no breakdown at caustics. The solution is still assumed to be of the form (2), but it is concentrated near a single ray of geometrical optics. To form such a solution, we first pick a ray and solve systems of ordinary differential equations (ODEs) along it to find the Taylor expansions of the phase and amplitude in variables transverse to the ray. Although the phase function is real-valued along the central ray, its imaginary part is chosen so that the solution decays exponentially away from the central ray, maintaining a Gaussian-shaped profile.

The existence of Gaussian beam solutions to the wave equation has been known since the 1960s, first in connection with lasers; see Babič and Buldyrev [2]. Later, they were used in the analysis of propagation of singularities in PDEs by Hörmander [20] and Ralston [38]. See also [4]. In the context of the Schrödinger equation, first order beams correspond to classical coherent states. Higher order versions of these have been introduced to approximate the Schrödinger equation in quantum chemistry by, e.g., Heller [15], Hagedorn [13], and Herman and Kluk [16].

More general high frequency solutions that are not necessarily concentrated on a single ray can be described by superpositions of Gaussian beams. This idea was first introduced by Babič and Pankratova in [3] and was later proposed as a method for approximating wave propagation by Popov in [40]. Letting the beam parameters depend on their initial location z such that $x = x(t; z)$, $p = p(t; z)$, etc., and $a = a(t, y; z)$, $\phi = \phi(t, y; z)$, the approximate solution for an initial value problem can be expressed with the superposition integral

$$(3) \qquad\qquad u(t, y) = \left(\frac{k}{2\pi}\right)^{\frac{d}{2}} \int_{K_0} a(t, y; z)e^{ik\phi(t,y;z)}dz,$$

where K_0 is a compact subset of $\mathbb{R}^d$.

Numerical methods based on Gaussian beam superpositions go back to the 1980s with work by Popov [40], Katchalov and Popov [26], Červený, Popov, and Pšenčík [9], and Klimeš [29] for high frequency waves and, e.g., Heller [15] and Herman and Kluk [16] in quantum chemistry. In the past decade there was a renewed interest in such methods for waves following their successful use in seismic imaging and oil exploration by Hill [17, 18]. Development of new beam based methods is now the subject of intense interest in the numerical analysis community, and the methods are being applied in a host of applications such as the original geophysical application [1, 31, 46], gravity waves [45], the semiclassical Schrödinger equation [12, 23, 30], and acoustic waves [44]. See also the survey of Gaussian beam methods in [22].

In this paper, we study the accuracy in terms of k of Gaussian beams and superpositions of Gaussian beams for the Helmholtz equation (1). This would give a rigorous foundation for beam based numerical methods used to solve the Helmholtz equation in the high frequency regime. In the time-dependent case several such error estimates have been derived in recent years: for the initial data [44], for scalar hyperbolic equations and the Schrödinger equation [33, 34, 35], for frozen Gaussians [42, 32], and for the acoustic wave equation with superpositions in phase space [5]. The general result is that the error between the exact solution and the Gaussian beam approximation decays as $k^{-N/2}$ for Nth order beams in the appropriate Sobolev norm. There are, however, no rigorous error estimates of this type available for the Helmholtz equation. What is known is how well the beams asymptotically satisfy the equation, i.e., the size of $L_n u$ for a single beam. Let us also mention an estimate of the Taylor expansion error away from caustics [37].

The analysis of Gaussian beam superpositions for the Helmholtz equation presents a few new challenges compared to the time-dependent case. First, it must be clarified precisely how beams are generated by the source function and how the Gaussian beam approximation is extended to infinity. This is done in sections 2 and 3 for a compactly supported source function that concentrates on a codimension one manifold. Second, additional assumptions on the index of refraction $n(x)$ are needed to get a well-posed problem with k-independent solution estimates and a well-behaved Gaussian beam approximation at infinity. The conditions we use are that $n(x)$ is nontrapping and that there is an R for which $n(x)$ is constant when $|x| > R$.

In section 4 we consider the difference between the Gaussian beam approximation $u_{GB}(x)$ and the exact solution $u(x)$ to the radiation problem with the corresponding source function. Here we are interested in behavior of the local Sobolev norms $||u_{GB} - u||_{H^s(|x|<R)}$ as $k \to \infty$. This depends on the well-posedness of the radiation problem. There are a variety of estimates that apply here [39, 7], but the Laplace-transform based estimates of Vainberg [47, 48] suffice for our purposes. In section 5, we compare the Gaussian beam approximation with the result of stationary phase expansion of the exact solution in a simple example.

Sections 6 and 7 are devoted to superpositions of beams with fundamental source terms. Our main result is Theorem 6.1, where we are able to show that the error between superposition of Nth order beams and the exact outgoing solution decays as $k^{-N/2}$ independent of dimension and presence of caustics. This is consistent with the optimal results of [35] in the time-dependent setting. Finally, section 7 gives an example of how beams can be constructed for more general source functions.

2. Construction of Gaussian beams. In this section we construct the Gaussian beam solutions for (1) when f is compactly supported on a codimension one manifold. This construction has become standard (see, for example, [38] or [27]) and we review some details here which will be used later. The form of the beam solutions is

$$(4) \qquad u(x;k) = e^{ik\phi(x)}(a_0(x) + a_1(x)k^{-1} + \cdots + a_\ell(x)k^{-\ell}).$$

Each beam concentrates on a geometrical optics ray $\gamma = \{x(s) : s \in \mathbb{R}\}$, which is the spatial part of the bicharacteristics $(x(s), p(s))$ defined by the flow for the Hamiltonian $H(x, p) = |p|^2 - n^2(x)$,

$$(5) \qquad\qquad \dot{x} = 2p, \quad \dot{p} = -\nabla_x n^2(x).$$

We assume that there is a number $R > 0$ such that the (smooth) index of refraction satisfies $n(x) \equiv 1$ when $|x| > R$ and that the source function f is compactly supported in $\{|x| < R\}$. Here we also restrict the construction of the Gaussian beam solution to the larger region $|x| \leq 6R$. The essential additional hypothesis for our construction is that the index of refraction does not lead to trapped rays. The precise nontrapping condition is that there is an L such that $|x(\pm L)| > 2R$ for all solutions with $|x(0)| < R$ and $H(x(0), p(0)) = 0$. Note that this implies that $|x(s)| > 2R$ for $|s| > L$ since rays are straight lines when $n(x) \equiv 1$. Some stronger forms of the nontrapping condition are found in the literature, for instance, the virial-like condition in [39, 6]. A simpler version of such a condition for (1) becomes $n(n - x \cdot \nabla n) \geq c > 0$, which can be shown to imply the nontrapping.

Applying L_n in (1) to (4), we have

$$(6) \qquad L_n u = e^{ik\phi} \sum_{j=-2}^{\ell} c_j(x) k^{-j},$$

where

$$c_{-2} = (n^2 - |\nabla_x \phi|^2) a_0 =_{def} E(x) a_0,$$
$$c_{-1} = i\alpha n^2 a_0 + \nabla_x \cdot (a_0 \nabla_x \phi) + \nabla_x a_0 \cdot \nabla_x \phi + E a_1,$$
$$c_j = i\alpha n^2 a_{j+1} + \nabla_x \cdot (a_{j+1} \nabla_x \phi) + \nabla_x a_{j+1} \cdot \nabla_x \phi + E a_{j+1} + \Delta_x a_j, \quad j = 0, 1, \ldots, \ell.$$

ODEs for $S(s) = \phi(x(s))$, $M(s) = D^2\phi(x(s))$, and $A_0(s) = a_0(x(s))$ arise from requiring that c_{-2} vanish to third order on the ray $x(s)$ and that c_{-1} vanish to first order on the ray. This leads to the equations

$$\dot{S} = 2n^2(x(s)),$$
$$(7) \qquad \dot{M} = D^2(n^2)(x(s)) - 2M^2,$$
$$\dot{A}_0 = -\text{tr}(M(s))A_0 - \alpha n^2(x(s))A_0.$$

This amounts to constructing a "first order" beam. Higher order beams can be constructed by requiring that c_{-2} vanish to higher order on γ. Then one can require that the c_j's with $j > -2$ also vanish to higher order and can obtain a recursive set of linear equations for the partial derivatives of $a_0, a_1, \ldots, a_\ell$. More precisely, for an Nth order beam, $\ell = \lceil N/2 \rceil - 1$ in (4) and $c_j(x)$ should vanish to order $N - 2j - 2$ when $-2 \leq j \leq \ell - 1$.

For initial data, we let $S(0) = 0$ and choose $M(0)$ so that

$$M(0) = M(0)^\top, \qquad M(0)\dot{x}(0) = \dot{p}(0), \qquad \text{Im}\{M(0)\} \text{ is positive definite on } \dot{x}(0)^\perp.$$

Then for all s the matrix $M(s)$ inherits the properties of $M(0)$: $M(s)\dot{x}(s) = \dot{p}(s)$, $M(s) = M(s)^\top$, and $\text{Im}\{M(s)\}$ is positive definite on the orthogonal complement of $\dot{x}(s)$; see [38]. For the amplitude we take $A_0(0) = 1$. We can solve the ODE for A_0 explicitly and obtain

$$A_0(s) = \exp\left(-\int_0^s (\alpha n^2(x(\tau)) + \text{tr}(M))d\tau\right).$$

The phase ϕ in (4) can be any function satisfying $\phi(x(s)) = S(s)$, $\nabla\phi(x(s)) = p(s)$, and $D^2\phi(x(s)) = M(s)$. However, to write such a function, we need to have s as
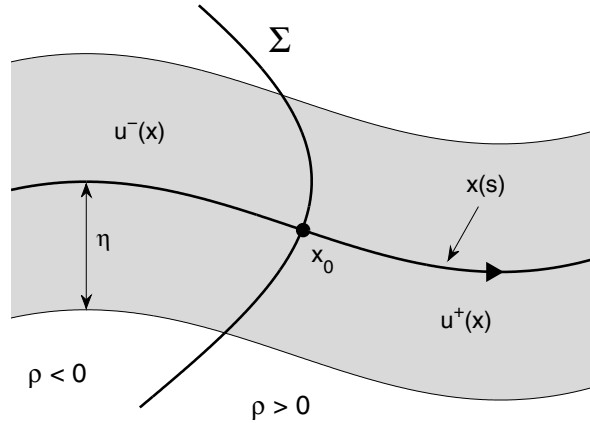
FIG. 1. *Notation for the source in two dimensions. The gray area indicates* $\Omega(\eta)$.

a function of x. Since we have $\dot{x}(s) \neq 0$, $x(s)$ traces a smooth curve γ in $\mathbb{R}^d$, and the nontrapping hypothesis implies that this curve is a straight line when $|s| > L$. We let

$$\Omega(\eta) = \{x \,:\, |x| \leq 6R \text{ and } |x - \gamma| \leq \eta\}$$

be the tubular neighborhood of γ with radius η in the ball $\{|x| \leq 6R\}$. By choosing η small enough, we can uniquely define $s = s(x)$ for all $x \in \Omega(\eta)$ such that $x(s)$ is the closest point on γ to x, provided γ has no self-intersections. (For the case of self-intersections, see Remark 2.1 below.) We then define the phase function ϕ and amplitude A on Ω for first order beams by

$$(8) \quad \phi(x) = S(s) + p(s) \cdot (x - x(s)) + \frac{1}{2}(x - x(s)) \cdot M(s)(x - x(s)), \qquad A(x) = A_0(s),$$

with $s = s(x)$. Note that $s(x)$ is constant on planes orthogonal to γ intersected with $\Omega(\eta)$. The construction of the Gaussian beam phase and amplitude for higher order beams is carried out in a similar way [38].

2.1. Source. To introduce the source functions that we will consider, we let ρ be a function such that $|\nabla \rho| = 1$ on $\{x : \rho(x) = 0\}$, and we define Σ to be the hypersurface $\{x : \rho(x) = 0\}$; see Figure 1. Given $x_0 \in \Sigma$, we let $(x(s), p(s))$ be the solution of (6) with $(x(0), p(0)) = (x_0, n(x_0)\nabla\rho(x_0))$. Since we assume no trapped rays and $n(x) \equiv 1$ when $|x| > R$, $x(s)$ and $p(s)$ are defined for $s \in \mathbb{R}$, and we set $\gamma = \{x(s), s \in \mathbb{R}\}$. Then we can assume that $s(x)$ is defined on the tubular neighborhood $\Omega(\eta)$ of γ as above (assuming no self-intersections). We begin with a beam $u(x, k)$ concentrated on γ and defined on $\Omega(\eta)$. If u is first order, we can define it by (8). Then we define u^+ to be the restriction of u to $\{x : \rho(x) \geq 0\}$. In order to have a source term which is a multiple of $\delta(\rho)$, we need a second beam $u^-(x, k)$ defined on $\{x : \rho(x) \leq 0\}$, which is equal to u^+ on Σ for all k. Hence, writing $u^+(x, k) = A^+(x, k)e^{ik\phi^+(x)}$ and $u^-(x, k) = A^-(x, k)e^{ik\phi^-(x)}$, we must have $\phi^+ = \phi^-$ and $A^+ = A^-$ on Σ. Those requirements and $c_j = 0$, $j = -2, \ldots, \ell$, at x_0 determine the Taylor series in the transverse variables at x_0 for ϕ^- and A^-. To see this suppose that u^- is going to be a beam of order N and that the coordinates on $\Omega(\eta)$ are given by (s, y), where $s = s(x)$

and $y = (y_1, \ldots, y_{d-1})$ is transversal. Then, provided η is chosen small enough, Σ is given by $s = \sigma(y)$ with $\sigma(0) = 0$ and $\nabla\sigma(0) = 0$. To determine the Taylor series in y for $\phi^-(s, y)$ at $s = 0$ one differentiates the equation $\phi^-(\sigma(y), y) = \phi^+(\sigma(y), y)$ with respect to y and evaluates at $y = 0$. When partial derivatives of ϕ^- with respect to s appear in this calculation, they are determined by the requirement that c_{-2} vanishes on $x(s)$ to order $N + 2$. The Taylor series for A^- in the transverse variables at x_0 is determined in the same way from $A^-(\sigma(y), y, k) = A^+(\sigma(y), y, k)$ for all k. To construct u^-, we use those Taylor series as data at $s = 0$ in solving the equations $c_j = 0$, $j = -2, \ldots, \ell$, along $x(s)$. Since for an Nth order beam we require only that c_j vanishes on $x(s)$ to order $N - 2j - 2$, we can still require that $\phi^+ = \phi^-$ and $A^+ = A^-$ *exactly* at points on Σ. Extending u^+ to be zero in $\{x : \rho(x) < 0\}$ and u^- to be zero in $\{x : \rho(x) > 0\}$, we define $u_{GB} = u^+ + u^-$. Then we have, setting $A = A^+ = A^-$ on Σ,

$$(9) \qquad L_n u_{GB} = \left[ik \left(\frac{\partial\phi^+}{\partial\nu} - \frac{\partial\phi^-}{\partial\nu} \right) A + \frac{\partial A^+}{\partial\nu} - \frac{\partial A^-}{\partial\nu} \right] e^{ik\phi^+} \delta(\rho) + f_{GB}$$

$$=_{def} g_0 \delta(\rho) + f_{GB},$$

where $\nu(x) = \nabla\rho(x)$, the unit normal to Σ. We consider the singular part of $L_n u_{GB}$ in (11), i.e., $g_0 \delta(\rho)$, to be the source term and f_{GB} to be the error from the Gaussian beam construction. Note that

$$(10) \qquad f_{GB} = e^{ik\phi^+(x)} \sum_{j=-2}^{\ell} c_j^+(x) k^{-j} + e^{ik\phi^-(x)} \sum_{j=-2}^{\ell} c_j^-(x) k^{-j},$$

where the $c_j^+(x)$ are extended to be zero when $\rho(x) < 0$ and the $c_j^-(x)$ are extended to be zero when $\rho(x) > 0$. For first order beams, $\ell = 0$ and (7) implies $c_{-2}^{\pm}(x)$ and $c_{-1}^{\pm}(x)$ are $O(|x - x(s(x))|^3)$ and $O(|x - x(s(x))|)$, respectively. Finally, we restrict the support of u_{GB} to $\Omega(\eta)$ by multiplying it by a smooth cutoff function $\varrho_\eta(x)$ supported in $\Omega(\eta)$ and identically equal to one on the smaller neighborhood $\Omega(\eta/2)$. The cutoff function modifies $A^{\pm}$ and f_{GB} outside $\Omega(\eta/2)$, but its contribution to (9) is exponentially small in k (see [35]), and we will disregard it from here on.

Remark 2.1. The nontrapping condition implies that all rays, γ, starting normal to Σ at $s = 0$ will be in $|x| > 2R$ for $|s| > L$. For $|s| \leq L$ all data (curvature, etc.) related to the rays range over compact sets. Hence, there is a $\delta > 0$ such that a self-intersection, $x(s_1) = x(s_2)$, implies $|s_1 - s_2| > \delta$, and there is an upper bound on the number of possible self-intersections for all ray paths considered here. Any γ can be cut into segments without self-intersections, and $s(x)$ is well-defined on a tubular neighborhood of each segment. The beam construction above can be done for s in each segment, continuing with consistent data across the endpoints of the segments, starting from the segments with endpoints on $s = 0$. Then there is a well-defined cutoff function on each segment for η sufficiently small, and we can choose η once for all γ considered here. So for the beam, we multiply each of the beams constructed for each segment by $\varrho_\eta(x)$ for that segment and add up these beams to get a beam for the entire ray path. Hence self-intersections will not create difficulties, and without loss of generality we will assume that γ has no self-intersections in what follows.

2.2. Estimate of f_{GB}. From the nontrapping condition, it follows that the length of a ray inside $\Omega(\eta)$ is bounded independently of the starting point in $|x| \leq R$.

By construction, $c_\ell^\pm(x)$ is bounded and

$$(11) \qquad c_j^\pm(x) = \sum_{|\beta|=N-2j-2} d_{\beta,j}^\pm(x)(x-x(s))^\beta, \qquad j = -2, \ldots, \ell-1,$$

where $d_{\beta,j}^\pm(x)$ are bounded on $\Omega(\eta)$; see, e.g., [33, pages 442–443] for a derivation of such c_j's. Hence,

$$|c_j^\pm(x)| \le C_j |x-x(s)|^{N-2j-2}, \qquad x \in \Omega(\eta).$$

Choosing η sufficiently small, the construction also ensures that

$$(12) \qquad \mathrm{Im}\{\phi^\pm\}(x) \ge c|x-x(s)|^2, \qquad x \in \Omega(\eta);$$

see [35]. From the bound

$$(13) \qquad s^p e^{-as^2} \le C_p a^{-p/2} e^{-as^2/2}, \qquad C_p = (p/e)^{p/2},$$

with $p = N - 2j - 2$, $a = kc$, and $s = |x-x(s)|$ we then get for $x \in \Omega(\eta)$,

$$|f_{GB}(x)| \le e^{-k\mathrm{Im}\{\phi^\pm\}(x)} \sum_{j=-2}^{\ell} |c_j^\pm(x)|k^{-j} \le e^{-kc|x-x(s)|^2} \sum_{j=-2}^{\ell} C_j |x-x(s)|^{N-2j-2}k^{-j}$$

$$(14) \qquad \le Ce^{-kc|x-x(s)|^2/2} \sum_{j=-2}^{\ell} k^{-N/2+j+1}k^{-j} \le Ce^{-kc|x-x(s)|^2/2}k^{-N/2+1}.$$

We note that the constant is uniform in $|x| \le 6R$, and in particular for first order beams, f_{GB} will be $O(k^{1/2}e^{-k\tilde{c}|x-x(s)|^2})$.

3. Extension of Gaussian beam solutions to infinity. In this section we extend $u_{GB}(x)$ defined on $|x| \le 6R$ to an outgoing solution $\tilde{u}_{GB}(x)$ in $\mathbb{R}^d$. For estimates on the validity of the approximation it is essential to do this so that

$$\tilde{f}_{GB} =_{def} L_n \tilde{u}_{GB} - g_0 \delta(\rho)$$

is supported in $|x| < 6R$ and is $o(k)$.

The main step in the extension is a simplified version of the procedure used in [36]. Let $G_\lambda(x)$ be the Green's function for the Helmholtz operator $\Delta + \lambda^2$, where λ may be complex-valued. When $\alpha \ge 0$, define

$$(15) \qquad k_\alpha := \sqrt{k^2 + ik\alpha}.$$

Then $L_1 = \Delta + i\alpha k + k^2 = \Delta + k_\alpha^2$, and G_{k_α} is uniquely determined when $\alpha > 0$ as the inverse of the self-adjoint operator L_1; for $\alpha = 0$ it can be defined either as $\lim_{\alpha \downarrow 0} G_{k_\alpha}$ or by radiation conditions. In the case $d = 3$,

$$G_{k_\alpha}(x) = -(4\pi)^{-1}\left(\frac{e^{ik_\alpha|x|}}{|x|}\right).$$

To extend u_{GB} we introduce the cutoff function $\eta_a(x)$ in $C^\infty(\mathbb{R}^d)$ with parameter $a \ge 1$:

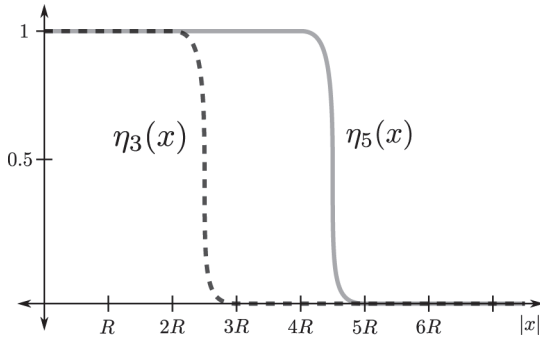$$\eta_a(x) = \begin{cases} 1 & |x| < (a-1)R, \\ 0 & |x| > aR \end{cases}$$

FIG. 2. *The cutoff functions $\eta_3(x)$ and $\eta_5(x)$.*

(see Figure 2) and define

$$(16) \qquad \tilde{u}_{GB} = \eta_3(x)u_{GB}(x) + \int G_{k_\alpha}(x-y)\eta_5(y)L_n[(1-\eta_3(y))u_{GB}(y)]dy.$$

We also assume that R is chosen large enough such that the support of $g_0\delta(\rho) \subset \Sigma \cap \Omega(\eta)$ is inside $\{|x| < R\}$.

Consider first $L_n\tilde{u}_{GB}$ in the region $\{|x| \geq R\}$. Since $L_n = L_1$ as well as $g_0\delta(\rho) = 0$ in this region and $\eta_5 \equiv 1$ on the support of η_3,

$$\tilde{f}_{GB}(x) = L_n\tilde{u}_{GB}(x) = \eta_5(x)L_n[\eta_3(x)u_{GB}(x)] + \eta_5(x)L_n[(1-\eta_3(x))u_{GB}(x)]$$
$$= \eta_5(x)L_n u_{GB} = \eta_5(x)f_{GB}(x).$$

Since η_5 is supported on $|x| < 5R$, it follows that $\tilde{f}_{GB}$ vanishes for $|x| > 5R$.

Consider next the region $\{|x| \leq R\}$, and let $v = \tilde{u}_{GB} - \eta_3 u_{GB}$, i.e., the integral term in (16). Since $\eta_3 = 1$ on $|x| < R$, we have in this region

$$\tilde{u}_{GB} - u_{GB} = v, \qquad \tilde{f}_{GB} - f_{GB} = L_n v.$$

In view of the estimate of f_{GB} it now suffices to show that for $|x| \leq R$, $\partial_x^\beta v$ decays rapidly when $k \to \infty$ for all multi-indices, $|\beta| \leq 2$.

By the definition of the two cutoff functions, we have for $|x| \leq R$

$$v(x) = \int_{\mathbb{R}^d} G_{k_\alpha}(x-y)\eta_5(y)L_n[(1-\eta_3(y))u_{GB}(y)]dy$$
$$= \int_{2R \leq |y| \leq 5R} G_{k_\alpha}(x-y)\eta_5(y)L_1[(1-\eta_3(y))u_{GB}(y)]dy.$$

The fundamental solution G_{k_α} has the form

$$G_{k_\alpha}(x) = \frac{e^{ik_\alpha|x|}}{|x|^{(d-1)/2}}w(x;k_\alpha),$$

where w and its derivatives in x are bounded by $|k_\alpha|^{\frac{d-3}{2}} \leq Ck^{\frac{d-3}{2}}$ on compact subsets of $|x| \geq R$; see the appendix. Since $n(x) \equiv 1$ for $|x| > R$, in that region, $x(s)$ is a straight line and $\nabla_x\phi^\pm(x(s))$ is a constant unit vector. Since $x(s)$ is going out of $|x| \leq R$ when it crosses $|x| = R$, at $x(s) = y$ with $|y| \geq 2R$ the phases in
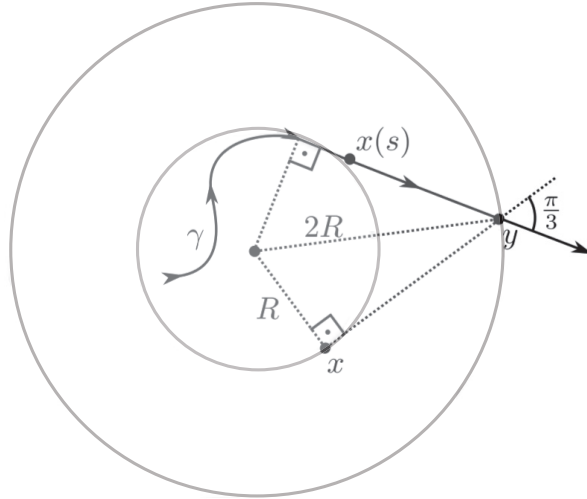
FIG. 3. *Maximum angle.*

u_{GB} satisfy $\nabla_x \phi^{\pm}(x(s)) \cdot y \geq \cos(\pi/6)|y|$. Likewise, when $|x| \leq R$ and $|y| \geq 2R$, $(y-x) \cdot y \geq |y||y-x| \cos(\pi/6)$ (see Figure 3). The form of u_{GB} (see (4)) gives the integrand in (16) the form $e^{ik\psi} b(y,k)$ with $\psi(y) = \phi^{\pm}(y) + (k_\alpha/k)|x-y|$ and b smooth in y, bounded together with its derivatives by $Ck^{\frac{d-3}{2}}$. Note that

$$\nabla_y \psi = \frac{k_\alpha}{k} \frac{y-x}{|y-x|} + \nabla_y \phi^{\pm}.$$

The preceding remarks show that, when $|x| \leq R$ and k is large, $\nabla_y \psi$ does not vanish on the support of the integrand in (16). Hence we can use the identity

$$e^{ik\psi} = \frac{\overline{\nabla_y \psi}}{ik|\nabla_y \psi|^2} \cdot \nabla_y (e^{ik\psi})$$

and integrate by parts to show that v and its derivatives are order k^{-m} for any m.

This completes the verification of the extension. We have shown that

(17) $\tilde{f}_{GB}(x) = \eta_5(x)[f_{GB}(x) + r(x)], \qquad ||r||_{L^2(|x|<5R)} = O(k^{-m}).$

Hence, the size of $\tilde{f}_{GB}$ is of the same order as the size of f_{GB}, which is of the order $O(k^{-N/2+1} e^{-k\tilde{c}|x-x(s)|^2})$. Moreover,

(18) $||u_{GB} - \tilde{u}_{GB}||_{H^s(|x|<R)} = O(k^{-m})$

for any m and s. Note that, since $\tilde{u}_{GB}$ is represented by $G_{\alpha,k}$ for $|x|$ large, it is square-integrable ($\alpha > 0$) or outgoing ($\alpha = 0$).

4. The error estimate for u_{GB}. In this section we will use an estimate showing that the radiation problem is well-posed due to Vainberg [47, 48]. This will give estimates on the accuracy of u_{GB} as an approximation to the exact solution in the region $|x| \leq R$. Vainberg starts with the initial value problem for the wave equation in $\mathbb{R}^d_x \times \mathbb{R}_t$,

$$v_{tt} - n^{-2}\Delta v = 0, \quad v(0) = 0, \quad v_t(0) = -n^{-2}g$$

and takes the Fourier–Laplace transform

$$(19) \qquad u(x, k) = \int_0^\infty e^{i\lambda t} v(t, x) dt$$

to get the solution to

$$\Delta u + \lambda^2 n^2 u = g$$

satisfying radiation conditions. Taking advantage of finite propagation speed, and the propagation of singularities to infinity, he estimates u on bounded regions from the integral representation (19) when g has bounded support and the nontrapping condition holds. In the notation of [47], $u = [\mathcal{R}_\lambda](n^{-2}g)$, where $\mathcal{R}_\lambda$ is the operator

$$\mathcal{R}_\lambda = (\lambda^2 + n^{-2}\Delta)^{-1}.$$

This is defined for complex λ as the analytic continuation of $\mathcal{R}_\lambda$ restricted to the space H_a^m with range in the space $H^m(|x| < b)$. The estimates take the following form: there are constants C and T such that

$$(20) \qquad ||\mathcal{R}_\lambda g||_{m+2-j,(b)} \le C|\lambda|^{1-j} e^{T|\operatorname{Im} \lambda|} ||g||_{m,a}, \quad 0 \le j \le 3.$$

Here the norms are standard Sobolev norms on $H_a^m(\mathbb{R}^d)$, the closure of $C_c^\infty(|x| < a)$ in $||\cdot||_m$, and $H^m(|x| < b)$. One can assume that $b < a$. The admissible set of λ here is the set

$$U_{c_1,c_2} = \{\lambda \in \mathbb{C} : |\operatorname{Im} \lambda| < c_1 \log |\operatorname{Re} \lambda| - c_2\}$$

for some $c_1, c_2 > 0$. If d is even, then one has to add the condition

$$-\pi/2 < \arg \lambda < 3\pi/2.$$

This is Theorem 3 for d odd and Theorem 4 for d even in [47].

Here we will apply (20) with $g = n^{-2}\tilde{f}_{GB}$, $a = 6R$, $b = R$, and $\lambda = k_\alpha \in \mathbb{C}$ with k_α defined as in (15). This makes $n^2 \mathcal{R}_{k_\alpha} g = \tilde{u}_{GB} - u_E$, where u_E is the exact solution to the radiation problem (1) with $f = g_0 \delta(\rho)$ defined as in (9). Taking $m = 0$ and $j = 0, 1, 2$, we have

$$(21) \qquad ||\tilde{u}_{GB} - u_E||_{H^{2-j}(|x|<R)} \le C|k_\alpha|^{1-j} e^{T|\operatorname{Im} k_\alpha|} ||\tilde{f}_{GB}||_{L^2}.$$

Note that $|k_\alpha| = k \left(1 + (\alpha/k)^2\right)^{1/4}$ and

$$|\operatorname{Im} k_\alpha| = \frac{\alpha}{\sqrt{2}} \left(\left(1 + (\alpha/k)^2\right)^{1/2} - 1\right)^{1/2}, \qquad |\operatorname{Re} k_\alpha| = \frac{k}{\sqrt{2}} \left(\left(1 + (\alpha/k)^2\right)^{1/2} + 1\right)^{1/2}.$$

Hence $|\operatorname{Im} k_\alpha| \le C$, $k_\alpha \in U_{c_1,c_2}$, for some $c_1, c_2 > 0$ and $|k_\alpha| > k$, so

$$(22) \qquad ||u_{GB} - u_E||_{H^{2-j}(|x|<R)} \le C|k|^{1-j} ||\tilde{f}_{GB}||_{L^2} + ||\tilde{u}_{GB} - u_{GB}||_{H^{2-j}(|x|<R)}$$

uniformly in terms of α. The estimates in (17) and (18) ensure that

$$(23) \qquad ||u_{GB} - u_E||_{H^j(|x|<R)} \le C|k|^{j-1} ||f_{GB}||_{L^2(|x|<5R)}, \qquad j = 0, 1, 2.$$

We observe here that since (17) and (18) hold uniformly for all beam starting points $x_0 \in \Sigma$, the estimate (23) will also hold for linear superpositions of beams, which we will discuss further below; see (33). Moreover, from (14) and the estimate (43) derived below, we obtain

$$||f_{GB}||^2_{L^2(|x|<5R)} \le Ck^{-N+2} \int_{\Omega(\eta)} e^{-2k\tilde{c}|x-x(s)|^2} dx \le Ck^{-N+2+(1-d)/2}.$$

This finally shows that for a single beam u_{GB},

$$||u_{GB} - u_E||_{H^j(|x|<R)} \le Ck^{-N/2-\sigma_d-j}, \qquad \sigma_d = \frac{d-1}{4}, \qquad j = 0, 1, 2.$$

Note that the factor $k^{-\sigma_d-j}$ corresponds to the size of the H^j norm of the beam itself in d dimensions, $||u_{GB}||_{H^j(|x|<R)} \sim k^{-\sigma_d-j}$, showing that the relative error of the beam in these norms is bounded by $k^{-N/2}$.

5. An example. Using the notation $x = (x_1, x') = (x_1, x_2, x_3)$, the outgoing solution to

$$\Delta u + k^2 u = 2ike^{-k|x'|^2/2}\delta(x_1)$$

is given by

$$(24) \qquad u(x, k) = \frac{-2ik}{4\pi} \int_{\mathbb{R}^2} \frac{e^{ik|x-(0,y')|-k|y'|^2/2}}{|x-(0,y')|} dy'.$$

In this section we compare the approximation that one gets by using the method of stationary phase on this integral to the approximation given by u_{GB}. The stationary phase approximation is not uniform in x', and for $x' \ne 0$ it simply gives $u(x_1, x', k) = O(k^{-N})$ for all N. However, when $x' = 0$, it gives $u_{GB}(x_1, 0)$.

The procedure for constructing u^+ given earlier with the source $2ike^{-|x'|^2/2}\delta(x_1)$ gives $x(s) = (2s, 0, 0)$, $p(s) = (1, 0, 0)$, $S(s) = 2s$, $M(s) = \frac{i}{1+2is}P$, and $A(s) = (1+2is)^{-1}$, where P is the orthogonal projection on $\hat{e}_1^\perp$. For u^- one gets the same results, with s replaced by $-s$ and $p(s)$ replaced by $-p(s)$. The definition of $s(x)$ gives $s(x) = |x_1|/2$, and we have

$$(25) \qquad u_{GB}(x, k) = (1 + i|x_1|)^{-1} e^{ik\phi}, \quad \text{where } \phi = |x_1| + \frac{i}{2(1+i|x_1|)}|y'|^2.$$

To apply the stationary phase lemma to (24) assume that $x_1 \ne 0$. Then the phase is given by $\psi(x, y') = |x-(0,y')| + i|y'|^2/2$, and we have

$$\psi_{y'} = \frac{y'-x'}{|x-(0,y')|} + iy',$$

which vanishes and is real only when $y' = x' = 0$. Then one has

$$\psi_{y'y'}|_{x'=y'=0} = \left(\frac{1}{|x_1|} + i\right) I_{2\times 2}.$$

The stationary phase lemma [21] gives

$$(26) \qquad u(x_1, 0) = \frac{2\pi}{k} (\det(-i\psi_{y'y'}(x_1)))^{-1/2} \left(\frac{-2ik}{4\pi} \frac{e^{ik|x_1|}}{|x_1|} + O(1)\right).$$

Since

$$\det(-i\psi_{y'y'}(x_1)) = \left(\frac{-i}{|x_1|} + 1\right)^2,$$

and the choice of square root leads to

$$\left(\left(\frac{-i}{|x_1|} + 1\right)^2\right)^{-1/2} = \left(\frac{-i}{|x_1|} + 1\right)^{-1},$$

one sees that the leading term in (26) is exactly (25).

6. Error estimates for superpositions. Given a point $z \in \Sigma$, we relabel the primitive source term g_0 in (9) as

$$(27) \qquad g(x, z, k) = [ik\zeta_1(x) + \zeta_2(x)]e^{-k|x-z|^2/2}\delta(\rho),$$

where $\zeta_j \in C_c^\infty$ and $\zeta_1(x) = 1$ on a neighborhood of $x = z$. Denoting the resulting beam as $u_{GB}(x; z)$, the error estimate (22) is uniform in z as long as z remains in a compact subset of $|x| < R$, for instance, $|z| \leq R/2$. If we let z range over Σ, we can form

$$(28) \qquad g(x, k)\delta(\rho) = \left(\frac{k}{2\pi}\right)^{(d-1)/2} \int_\Sigma g(x, z, k)h(z)dA_z,$$

and

$$(29) \qquad u(x) = \left(\frac{k}{2\pi}\right)^{(d-1)/2} \int_\Sigma u_{GB}(x; z)h(z)dA_z$$

is an approximation to the exact solution for the source $g(x, k)\delta(\rho)$ satisfying the estimate (22).

We now state the main result of error estimates for superposition (29).

THEOREM 6.1. *Assume that $n(x)$ is smooth, nontrapping, positive, and equal to 1 when $|x| > R$. Let u_E be the exact solution to (1) with the source $f = g(x, k)\delta(\rho)$ in (28), and let u be the Gaussian beam superposition defined in (29) based on Nth order beams. We then have the estimate*

$$(30) \qquad \|u - u_E\|_{H^m(|x| \leq R)} \leq Ck^{-N/2+m}, \qquad m = 0, 1, 2,$$

where C is independent of k but may depend on R.

We proceed to complete the proof of this theorem by following the same general steps as in the proof of [35, Theorem 1.1]. The main difference in this part is a modified version of the "nonsqueezing" lemma, Lemma 6.2, in which two trajectories in phase space are shown to be close if their initial points on the source are close. The way distance between beams is measured here must be allowed to vary smoothly with the observation point and the beam's initial point. Another improvement is the way the integration below is split into two cases in (37), corresponding to regions away from and close to caustics.

In order to simplify the notation, we specify $\rho(x) = x_1$ and $y = (0, z)$ for $z \in \Sigma \subset \mathbb{R}^{d-1}$. The superposition thus can be written as

$$(31) \qquad u(x) = \left(\frac{k}{2\pi}\right)^{(d-1)/2} \int_\Sigma u_{GB}(x; z)h(z)dz,$$

and the residual

$$(32) \qquad L_n u - L_n u_E = f(x) = \left(\frac{k}{2\pi}\right)^{(d-1)/2} \int_\Sigma f_{GB}(x; z) h(z) dz.$$

By the definition of u_E and the source $g(x, k)\delta(\rho)$, the residual f contains only regular terms. We can therefore extend the superposition u to $\tilde{u}$ in the same way as in section 3 and define $\tilde{f} = L_n \tilde{u} - L_n u_E$. As observed above, (17) and (18) hold uniformly for all $z \in \Sigma$, and the same steps as in section 4 therefore lead to an estimate corresponding to (23), namely,

$$(33) \qquad ||u - u_E||_{H^m(|x| \le R)} \le C k^{m-1} ||f||_{L^2(|x| < 5R)}, \qquad m = 0, 1, 2.$$

We let $x(s; z)$ be the ray originating in z, $x(0, z) = z$, and we denote by $\Omega(\eta; z)$ the corresponding tubular neighborhood of radius η in the ball $\{|x| \le 5R\}$. By choosing $\eta > 0$ sufficiently small, we can thus ensure that $s = s(x; z)$ is well-defined on $\Omega(\eta; z)$. In what follows we denote $x(s(x, z); z)$ by γ or $\gamma(x; z)$. Moreover, we introduce the cutoff function $\varrho_\eta(x) \in C^\infty(\mathbb{R}^d)$ as

$$(34) \qquad \varrho_\eta(x) \ge 0 \quad \text{and} \quad \varrho_\eta(x) = \begin{cases} 1 \text{ for } |x| \le \eta/2, \\ 0 \text{ for } |x| \ge \eta \end{cases}$$

such that $\varrho_\eta(x - \gamma(x; z))$ is supported on $\Omega(\eta; z)$ and is identically equal to one on $\Omega(\eta/2; z)$. The form (10) of $f_{GB}(x; z)$ will then be

$$f_{GB}(x; z) = \left(e^{ik\phi^+(x;z)} \sum_{j=-2}^{\ell} c_j^+(x; z) k^{-j} \right.$$

$$\left. + e^{ik\phi^-(x;z)} \sum_{j=-2}^{\ell} c_j^-(x; z) k^{-j} \right) \varrho_\eta(x - \gamma) + O(k^{-\infty})$$

$$= \sum_\alpha k^{j_\alpha} e^{ik\phi_\alpha(x;z)} d_\alpha(x; z) (x - \gamma)^{\beta_\alpha} \varrho_\eta(x - \gamma) + O(k^{-\infty}),$$

with bounds

$$|\beta_\alpha| \le N + 2, \qquad 2j_\alpha \le 2 - N + |\beta_\alpha|.$$

The sum over α is finite, d_α involves the functions $d_{\beta,j}^\pm$ in (11), and ϕ_α is either ϕ^+ or ϕ^-. Moreover, $O(k^{-\infty})$ indicates terms exponentially small in $1/k$. After neglecting these terms and using (32) it follows that we can bound the L^2 norm of f by

$$||f||_{L^2(|x| \le 5R)}^2 \le C k^{d-1} \sum_\alpha \left\| \int_\Sigma k^{\frac{2-N+|\beta_\alpha|}{2}} e^{ik\phi_\alpha} d_\alpha (x - \gamma)^{\beta_\alpha} \varrho_\eta h dz \right\|_{L^2(|x| \le 5R)}^2$$

$$= C k^{d-N} \sum_\alpha \int_{|x| \le 5R} \int_\Sigma \int_\Sigma I_\alpha(x, z, z') dz dz' dx,$$

where the terms I_α are of the form

$$I_\alpha(x, z, z') = k^{1+|\beta|} e^{ik\psi(x,z,z')} g(x; z') \overline{g(x; z)}$$

$$\times (x - \gamma)^\beta (x - \gamma')^\beta \varrho_\eta(x - \gamma) \varrho_\eta(x - \gamma'), \quad |\beta| \le 3.$$

Here $g(x; z) = d_\alpha(x; z) h(z)$ and

$$(35) \qquad \psi(x, z, z') := \phi(x; z') - \overline{\phi(x; z)},$$

with ϕ being either of $\phi^\pm$. The function g and its derivatives are bounded,

$$(36) \qquad \sup_{z \in \Sigma, x \in \Omega(\eta; z)} |\partial_x^\lambda g(x; z)| \leq C_\lambda,$$

for any $|\lambda| \geq 0$.

Let $\chi_j(x, z, z') \in C^\infty$ be a partition of unity such that

$$(37) \qquad \chi_1(x, z, z') = \begin{cases} 1 & \text{when } |\gamma(x, z) - \gamma(x, z')| > \theta |z - z'|, \\ 0 & \text{when } |\gamma(x, z) - \gamma(x, z')| < \frac{1}{2}\theta |z - z'|, \end{cases}$$

and $\chi_1 + \chi_2 = 1$. Moreover, let

$$I_1 = \chi_1(x, z, z') I_\alpha(x, z, z'), \qquad I_2 = \chi_2(x, z, z') I_\alpha(x, z, z'),$$

so that $I_\alpha(x, z, z') = I_1 + I_2$.

The rest of this section is dedicated to establishing the inequality

$$(38) \qquad \left| \int_{|x| \leq 5R} \int_\Sigma \int_\Sigma I_j(x, z, z') \, dx \, dz \, dz' \right| \leq C k^{2-d}$$

for $j = 1, 2$. With this estimate we have $\|f\|_{L^2(|x| \leq 5R)} \leq C k^{1-N/2}$, which together with (33) lead to the desired estimate (30).

A key ingredient in establishing estimate (38) is a slight generalization of the nonsqueezing lemma obtained in [35]. It says that the distance in phase space between two smooth Hamiltonian trajectories at two parameter values s that depends smoothly on the initial position z will not shrink from its initial distance, even in the presence of caustics. The lemma is as follows.

LEMMA 6.2 (nonsqueezing lemma). *Let* $X = (x(s; z), p(s; z))$ *be the bicharacteristics starting from* $z \in \Sigma$ *with* Σ *bounded. Assume that* $p(0; z) \in C^2(\Sigma)$ *is perpendicular to* Σ *for all* z*, that* $|p(0; z)| = n(z)$*, and that* $\inf_z n(z) = n_0 > 0$*. Let* $S(z)$ *be a Lipschitz continuous function on* Σ *with Lipschitz constant* S_0*. Then, there exist positive constants* c_1 *and* c_2 *depending on* L*,* S_0*, and* n_0 *such that*

$$(39) \qquad c_1 |z - z'| \leq |p(S(z); z) - p(S(z'); z')| \\ + |x(S(z); z) - x(S(z'); z')| \leq c_2 |z - z'|$$

for all $z, z' \in \Sigma$ *and* $|S(z)|, |S(z')| \leq L$*.*

Proof. With the assumptions given here, the nonsqueezing lemma proved in [35] states that there are positive constants $0 < d_1 \leq d_2$ such that

$$(40) \qquad d_1 |z - z'| \leq |p(s; z) - p(s; z')| + |x(s; z) - x(s; z')| \leq d_2 |z - z'|$$

for all $z, z' \in \Sigma$ and $|s| \leq L$, i.e., essentially the case $S(z) \equiv$ constant. Since the Hamiltonian for the flow (5) is regular for all p, x, and the initial data $p(0; z)$ are $C^2(\Sigma)$, the derivatives $\partial_{s,z}^\alpha x$ and $\partial_{s,z}^\alpha p$ with $|\alpha| \leq 2$ are all bounded on $[-L, L] \times \Sigma$ by

a constant M. Then, for the right inequality in (39), we have

$$|p(S(z); z) - p(S(z'); z')| + |x(S(z); z) - x(S(z'); z')|$$
$$\leq |p(S(z); z) - p(S(z'); z)| + |p(S(z'); z) - p(S(z'); z')|$$
$$+ |x(S(z); z) - x(S(z'); z)| + |x(S(z'); z) - x(S(z'); z')|$$
$$\leq 2M|S(z) - S(z')| + d_2|z - z'| \leq (2MS_0 + d_2)|z - z'| =: c_2|z - z'|$$

by (40) and the Lipschitz continuity of $S(z)$. For the left inequality in (39),

$$(41) \quad |x(S(z); z) - x(S(z'); z')| + |p(S(z); z) - p(S(z'); z')|$$
$$\geq |p(S(z); z) - p(S(z); z')| - |p(S(z); z') - p(S(z'); z')|$$
$$+ |x(S(z); z) - x(S(z); z')| - |x(S(z); z') - x(S(z'); z')|$$
$$\geq d_1|z - z'| - |p(S(z); z') - p(S(z'); z')| - |x(S(z); z') - x(S(z'); z')|$$
$$\geq d_1|z - z'| - 2M|S(z) - S(z')|,$$

where we again used (40). Next we will estimate $|S(z) - S(z')|$ using $|x(S(z'); z') - x(S(z); z)|$. From Taylor expansion of x around z, and the fact that $x_s = 2p$, we have

$$x(S(z'); z') - x(S(z); z) = 2p(S(z); z)(S(z) - S(z')) + D_z x(S(z); z)(z' - z) + R(z, z'),$$

where

$$(42) \quad |R(z, z')| \leq M\left(|S(z) - S(z')|^2 + |z - z'|^2\right) \leq M(1 + S_0^2)|z - z'|^2.$$

Moreover,

$$\frac{d}{ds} p(s; z)^T D_z x(s; z) = p_s(s; z)^T D_z x(s; z) + p(s; z)^T D_z x_s(s; z)$$
$$= -\nabla_x n^2(x(s; z))^T D_z x(s; z) + 2p(s; z)^T D_z p(s; z)$$
$$= \nabla_z H(x(s; z), p(s; z)) = \nabla_z H(x(0; z), p(0; z)) = 0$$

by the choice of data at $s = 0$. Therefore, since $p(0; z)$ is orthogonal to Σ and $x_{z_j}(0; z)$ are tangent vectors to Σ, we have $p(s; z)^T D_z x(s; z) = 0$ for all s and

$$|x(S(z); z) - x(S(z'); z')| \geq 2|p(S(z); z)||S(z) - S(z')| - |R| \geq 2n_0|S(z) - S(z')| - |R|.$$

This estimate, together with (41) and (42), now gives

$$|x(S(z); z) - x(S(z'); z')| + |p(S(z); z) - p(S(z'); z')|$$
$$\geq d_1|z - z'| - \frac{M}{n_0}|x(S(z); z) - x(S(z'); z')| - \frac{M^2(1 + S_0^2)}{n_0}|z - z'|^2,$$

which implies

$$|x(S(z); z) - x(S(z'); z')| + |p(S(z); z) - p(S(z'); z')| \geq \tilde{d}_1|z - z'|\left(1 - m|z - z'|\right),$$

with $m = M^2(1 + S_0^2)/(n_0 d_1)$ and $\tilde{d}_1 = d_1/(1 + M/n_0)$. The lemma is thus proved for $|z - z'| \leq 1/2m$ with $c_1 = \tilde{d}_1/2$. On the other hand, if $|z - z'| \geq 1/2m$, there is a number $c(m)$ such that

$$\inf_{\substack{z, z' \in \Sigma, \ |z-z'| \geq 1/2m \\ |s| \leq L, \ |s'| \leq L}} |p(s; z) - p(s'; z')| + |x(s; z) - x(s'; z')| =: c(m) > 0$$

by the uniqueness of solutions to the Hamiltonian system. Hence, in particular, for $|z - z'| \geq 1/2m$,

$$|x(S(z); z) - x(S(z'); z')| + |p(S(z); z) - p(S(z'); z')| \geq c(m) \geq \frac{c(m)}{\Lambda}|z - z'|,$$

where $\Lambda = \sup_{z,z' \in \Sigma} |z - z'| < \infty$ is the diameter of the bounded set Σ. This proves the lemma with $c_1 = \min(\tilde{d}_1/2, c(m)/\Lambda)$.   □

We now prepare some main estimates for proving (38).

LEMMA 6.3 (phase estimates). *Let η be small and $x \in D(\eta, z, z')$, where*

$$D(\eta, z, z') = \Omega(\eta, z) \cap \Omega(\eta, z').$$

- *For all $z, z' \in \Sigma$ and sufficiently small η, there exists a constant δ independent of k such that*

$$\Im\psi(x, z, z') \geq \delta\left[|x - \gamma|^2 + |x - \gamma'|^2\right].$$

- *For $|\gamma(x; z) - \gamma(x; z')| < \theta|z - z'|$,*

$$|\nabla_x\psi(x, z, z')| \geq C(\theta, \eta)|z - z'|,$$

  where $C(\theta, \eta)$ is independent of x and positive if θ and η are sufficiently small.

Proof. The first result follows directly from (12). For the second result, we obtain

$$\begin{aligned}|\nabla_x\psi(x, z, z')| &\geq |\Re\nabla_x\psi(x, z, z')|\\ &= |\Re\nabla_x\phi(x; z') - \Re\nabla_x\phi(x; z)|, \qquad \left\{h := \Re\nabla_x\phi\right\}\\ &= \Big|h(\gamma'; z') - h(\gamma; z) + h(\gamma; z') - h(\gamma'; z')\\ &\quad + h(x; z') - h(\gamma; z') + h(\gamma, z) - h(x, z)\Big|.\end{aligned}$$

For the function $z \mapsto s(x; z)$ we can find a Lipschitz constant that is uniform in x. Recalling that $\gamma = x(s(x; z); z)$ and $\gamma' = x(s(x; z'); z')$, we can therefore use (39) in Lemma 6.2 for the first pair and obtain

$$|h(\gamma'; z') - h(\gamma; z)| = |p(s(x; z'); z') - p(s(x; z); z)| \geq c_1|z - z'| - |\gamma - \gamma'|.$$

The second pair $|h(\gamma; z') - h(\gamma'; z')|$ is bounded by $C_1|\gamma - \gamma'|$. Then, by the fundamental theorem of calculus, for $x \in D(\eta, z, z')$, the remaining terms are

$$\left|\int_0^1 \left[D^2\phi(\tau x + (1 - \tau)\gamma; z') - D^2\phi(\tau x + (1 - \tau)\gamma; z)\right](x - \gamma)d\tau\right|$$
$$\leq C|z - z'||x - \gamma| \leq C_2\eta|z - z'|.$$

Using these estimates for the case $|\gamma - \gamma'| < \theta|z - z'|$, we then obtain

$$\begin{aligned}|\nabla_x\psi(x, z, z')| &\geq c_1|z - z'| - |\gamma - \gamma'| - C_1|\gamma - \gamma'| - C_2\eta|z - z'|\\ &\geq c_1|z - z'| - (1 + C_1)\theta|z - z'| - C_2\eta|z - z'|\\ &=: C(\theta, \eta)|z - z'|\end{aligned}$$

where $C(\theta, \eta)$ is positive if θ and η are small enough.   □

6.1. Estimate of I_1. We start by looking at I_1, which corresponds to the non-caustic region of the solution. We have

$$\mathcal{I}_1 := \left| \int_{|x| \leq 5R} \int_\Sigma \int_\Sigma I_1(x, z, z') dz dz' dx \right|$$

$$\leq k^{1+|\beta|} \int_\Sigma \int_\Sigma \int_{D(\eta, z, z')} \chi_1(x, z, z') e^{ik\psi(x, z, z')} g(x; z') \overline{g(x; z)}$$

$$\times (x - \gamma)^\beta (x - \gamma')^\beta \varrho_\eta(x - \gamma) \varrho_\eta(x - \gamma') dx dz dz'.$$

We begin estimating

$$|\mathcal{I}_1| \leq C k^{1+|\beta|} \int_\Sigma \int_\Sigma \int_{D(\eta, z, z')} \chi_1(x, z, z') |x - \gamma|^{|\beta|} |x - \gamma'|^{|\beta|} e^{-\delta k(|x-\gamma|^2 + |x-\gamma'|^2)} dx dz dz'.$$

Now, using the estimate (13) with $p = |\beta|$, $a = \delta k$, and $s = |x - \gamma|$ or $|x - \gamma'|$, and continuing the estimate of I_1, we have for a constant, C, independent of z and z',

$$|\mathcal{I}_1| \leq C k^{|\beta|+1} \left(\frac{1}{k\delta} \right)^{|\beta|} \int_\Sigma \int_\Sigma \int_{D(\eta, z, z')} \chi_1(x, z, z') e^{-\frac{\delta k}{2}(|x-\gamma|^2 + |x-\gamma'|^2)} \, dx dz dz'$$

$$\leq C k \int_\Sigma \int_\Sigma \int_{D(\eta, z, z')} \chi_1(x, z, z') e^{-\frac{\delta k}{4}(|x-\gamma|^2 + |x-\gamma'|^2)} e^{-\frac{\delta k}{8}|\gamma-\gamma'|^2} e^{-\frac{\delta k}{2}|x-\bar{\gamma}|^2} \, dx dz dz'$$

$$\leq C k \int_\Sigma \int_\Sigma \int_{D(\eta, z, z')} \chi_1(x, z, z') e^{-\frac{\delta k}{4}(|x-\gamma|^2 + |x-\gamma'|^2)} e^{-\frac{\delta k}{8}|\gamma-\gamma'|^2} \, dx dz dz'$$

$$\leq C k \int_\Sigma \int_\Sigma e^{-\frac{\delta k}{8}\theta|z-z'|^2} \int_{D(\eta, z, z')} e^{-\frac{\delta k}{4}(|x-\gamma|^2 + |x-\gamma'|^2)} \, dx dz dz'.$$

Here we have used the identity

$$|x - \gamma|^2 + |x - \gamma'|^2 = 2|x - \bar{\gamma}|^2 + \frac{1}{2}|\gamma - \gamma'|^2$$

and the fact that $|\gamma - \gamma'| > \frac{1}{2}\theta|z - z'|$ on the support of χ_1. For the inner integral we can use the Cauchy–Schwarz inequality, together with the fact that $D \subset \Omega(\eta; z)$ and $D \subset \Omega(\eta; z')$,

$$\int_{D(\eta, z, z')} e^{-\frac{\delta k}{4}(|x-\gamma|^2 + |x-\gamma'|^2)} dx \leq \left(\int_{\Omega(\eta; z)} e^{-\frac{\delta k}{2}(|x-\gamma|^2)} dx \int_{\Omega(\eta; z')} e^{-\frac{\delta k}{2}(|x-\gamma'|^2)} dx \right)^{1/2}.$$

By a change of local coordinates, we can show that

$$(43) \qquad \int_{\Omega(\eta; z)} e^{-\frac{\delta k}{4}|x-\gamma|^2} \, dx \leq C k^{(1-d)/2}.$$

From this it follows that

$$(44) \qquad |\mathcal{I}_1| \leq C k^{(3-d)/2} \int_\Sigma \int_\Sigma e^{-\frac{\delta k}{8}\theta|z-z'|^2} \, dz dz'.$$

To show (43) for each z, we introduce local coordinates in the tubular neighborhood $\Omega(\eta; z)$ around the ray γ in the following way: choose (smoothly in (s, z)) a normalized

orthogonal basis $e_1(s, z), \ldots, e_{d-1}(s, z)$ in the plane $\{x : (x - x(s; z)) \cdot p(s; z) = 0\}$ with the origin at $x(s; z)$. Since s and z lie in compact sets, there will be an $\eta > 0$ such that in the tube $\Omega(\eta; z)$ the mapping from x to (s, y) defined by

$$x = x(s; z) + y_1 e_1(s, z) + \cdots + y_{d-1} \cdot e_{d-1}(s, z)$$

will be a diffeomorphism depending smoothly on z, and hence

$$\int_{\Omega(\eta; z)} e^{-\frac{\delta k}{4} |x - \gamma|^2} \, dx = \int_{|s| \leq L_0} \int_{|y| \leq \eta} e^{-\frac{\delta k}{4} |y|^2} \left| \frac{\partial x}{\partial (y, s)} \right| dy ds \leq Ck^{(1-d)/2},$$

where L_0 is chosen such that $|x(L_0; z)| \geq 5R$ for all $z \in \Sigma$. Letting $\Lambda = \sup_{z, z' \in \Sigma} |z - z'| < \infty$ be the diameter of Σ, we continue to estimate the (z, z')-integral left in (44):

$$\begin{aligned}
|\mathcal{I}_1| &\leq Ck^{(3-d)/2} \int_{\Sigma} \int_{\Sigma} e^{-\frac{\delta k}{8} \theta |z - z'|^2} \, dz dz' \\
&\leq Ck^{(3-d)/2} \int_0^{\Lambda} \tau^{d-2} e^{-\frac{k \delta \theta^2}{8} \tau^2} d\tau \\
&\leq Ck^{2-d},
\end{aligned}$$

which concludes the estimate of I_1.

6.2. Estimate of I_2. In order to estimate I_2 we use a version of the nonstationary phase lemma (see [21]).

LEMMA 6.4 (nonstationary phase lemma). *Suppose that $u(x; \zeta) \in C_0^\infty(\Omega \times Z)$, where Ω and Z are compact sets and $\psi(x; \zeta) \in C^\infty(O)$ for some open neighborhood O of $\Omega \times Z$. If $\nabla_x \psi$ never vanishes in O, then for any $K = 0, 1, \ldots,$*

$$\left| \int_\Omega u(x; \zeta) e^{ik\psi(x;\zeta)} dx \right| \leq C_K k^{-K} \sum_{|\lambda| \leq K} \int_\Omega \frac{|\partial_x^\lambda u(x; \zeta)|}{|\nabla_x \psi(x; \zeta)|^{2K - |\lambda|}} e^{-k \Im \psi(x;\zeta)} dx,$$

where C_K is a constant independent of ζ.

We now define

$$\begin{aligned}
\tilde{I}_2(z, z') &:= \int_{|x| \leq 5R} I_2(x, z, z') dx \\
&= k^{1+|\beta|} \int_{D(\eta, z, z')} \chi_2(x, z, z') e^{ik\psi(x, z, z')} g(x; z') \overline{g(x; z)} \\
&\quad \times (x - \gamma)^\beta (x - \gamma')^\beta \varrho_\eta(x - \gamma) \varrho_\eta(x - \gamma') dx.
\end{aligned}$$

In this case, Lemma 6.4 can be applied to $\tilde{I}_2$ with $\zeta = (z, z') \in \Sigma \times \Sigma$ to give

$$\left|\tilde{I}_2\right| \leq C_K k^{1+|\beta|-K} \sum_{|\lambda| \leq K} \int_{D(\eta, z, z')} \frac{\left|\partial_x^\lambda \left[(x-\gamma)^\beta (x-\gamma')^\beta \chi_2 g' \overline{g} \varrho_\eta \varrho_\eta'\right]\right|}{|\nabla_x \psi(x, z, z')|^{2K-|\lambda|}} e^{-\Im k\psi(x, z, z')} dx$$

$$\leq C_K k^{1+|\beta|-K} \sum_{|\lambda| \leq K} \left(\frac{1}{(C(\theta, \eta)|z - z'|)^{2K-|\lambda|}} \right.$$

$$\times \int_{D(\eta, z, z')} \left|\partial_x^\lambda \left[(x-\gamma)^\beta (x-\gamma')^\beta \chi_2 g' \overline{g} \varrho_\eta \varrho_\eta'\right]\right| e^{-\Im k\psi} dx \Bigg)$$

$$\leq C_K k^{1+|\beta|-K} \sum_{|\lambda| \leq K} \frac{1}{|z - z'|^{2K-|\lambda|}} \left(\sum_{\substack{\lambda_1+\lambda_2=\lambda \\ \lambda_1 \leq 2\beta}} \int_{D(\eta, z, z')} \left|\partial_y^{\lambda_1} \left[(x-\gamma)^\beta (x-\gamma')^\beta\right]\right| \right.$$

$$\times \left|\partial_x^{\lambda_2} \left[\chi_2 g' \overline{g} \varrho_\eta \varrho_\eta'\right]\right| e^{-\Im k\psi} dx \Bigg) ,$$

where $\varrho_\eta' = \varrho_\eta(x-\gamma')$, and we used the fact that $|\nabla_x \psi(x, z, z')| \geq C(\theta, \eta)|z - z'|$ on the support of χ_2, shown in Lemma 6.3. The constant C_K is independent of z and z'. By the bound (36), since ϱ_η is uniformly smooth, and x, z, z' vary in a compact set, $\left|\partial_x^{\lambda_2} \left[\chi_2 g' \overline{g} \varrho_\eta \varrho_\eta'\right]\right|$ can be bounded by a constant independent of x, z, and z'. We estimate the other term as follows:

$$\left|\partial_x^{\lambda_1} \left[(x-\gamma)^\beta (x-\gamma')^\beta\right]\right| \leq C \sum_{\substack{\lambda_{11}+\lambda_{12}=\lambda_1 \\ \lambda_{11}, \lambda_{12} \leq \beta}} \left|(x-\gamma)^{\beta-\lambda_{11}} (x-\gamma')^{\beta-\lambda_{12}}\right|$$

$$\leq C \sum_{\substack{\lambda_{11}+\lambda_{12}=\lambda_1 \\ \lambda_{11}, \lambda_{12} \leq \beta}} |x-\gamma|^{|\beta|-|\lambda_{11}|} |x-\gamma'|^{|\beta|-|\lambda_{12}|} .$$

Now, using the same argument as for estimating I_1, we have

$$\int_{D(\eta, z, z')} \left|\partial_y^{\lambda_1} \left[(x-\gamma)^\beta (x-\gamma')^\beta\right]\right| \left|\partial_y^{\lambda_2} \left[\chi_2 g' \overline{g} \varrho_\eta \varrho_\eta'\right]\right| e^{-\Im k\psi} dx$$

$$\leq C \sum_{\substack{\lambda_{11}+\lambda_{12}=\lambda_1 \\ \lambda_{11}, \lambda_{12} \leq \beta}} \int_{D(\eta, z, z')} |x-\gamma|^{|\beta|-|\lambda_{11}|} |x-\gamma'|^{|\beta|-|\lambda_{12}|} e^{-\Im k\psi} dx$$

$$\leq C(\lambda_2) k^{\frac{-|\beta|+|\lambda_{11}|-|\beta|+|\lambda_{12}|}{2}} \int_{D(\eta, z, z')} e^{-\frac{k\delta}{2}((x-\gamma)^2+(x-\gamma')^2)} dx$$

$$\leq C k^{(1-d)/2-|\beta|+|\lambda_1|/2} ,$$

and consequently,

$$\left|\tilde{I}_2\right| \leq C_K k^{1+|\beta|-K} \sum_{|\lambda| \leq K} \frac{1}{|z - z'|^{2K-|\lambda|}} \sum_{\substack{\lambda_1+\lambda_2=\lambda \\ \lambda_1 \leq 2\beta}} C(\lambda_2) k^{(1-d)/2-|\beta|+|\lambda_1|/2}$$

$$\leq C_K k^{(3-d)/2} \sum_{|\lambda| \leq K} \frac{1}{(|z - z'|\sqrt{k})^{2K-|\lambda|}} .$$

On the support of χ_2 the difference $|z - z'|$ can be arbitrary small, in which case this estimate is not useful. However, it is easy to check that the estimate is true also for

$K = 0$, and $\tilde{I}_2$ is thus bounded by the minimum of the $K = 0$ and $K > 0$ estimates. Therefore,

$$
\left| \tilde{I}_2 \right| \le C k^{(3-d)/2} \min \left[1, \sum_{|\lambda| \le K} \frac{1}{\left(|z - z'| \sqrt{k} \right)^{2K - |\lambda|}} \right]
$$

$$
\le C k^{(3-d)/2} \sum_{|\lambda| \le K} \min \left[1, \frac{1}{\left(|z - z'| \sqrt{k} \right)^{2K - |\lambda|}} \right]
$$

$$
\le C k^{(3-d)/2} \sum_{|\lambda| \le K} \frac{1}{1 + \left(|z - z'| \sqrt{k} \right)^{2K - |\lambda|}} \le C \frac{k^{(3-d)/2}}{1 + \left(|z - z'| \sqrt{k} \right)^K} \ .
$$

Finally, letting $\Lambda = \sup_{z, z' \in \Sigma} |z - z'| < \infty$ be the diameter of Σ, we compute

$$
\int_{\Sigma \times \Sigma} \left| \tilde{I}_2(z, z') \right| dz dz' \le C k^{\frac{3-d}{2}} \int_{\Sigma \times \Sigma} \frac{1}{1 + \left(|z - z'| \sqrt{k} \right)^K} dz dz'
$$

$$
\le C k^{\frac{3-d}{2}} \int_0^\Lambda \frac{1}{1 + (\tau \sqrt{k})^K} \tau^{d-2} d\tau
$$

$$
\le C k^{2-d} \int_0^\infty \frac{\xi^{d-2}}{1 + \xi^K} d\xi
$$

$$
\le C k^{2-d}
$$

if we take $K > d - 1$. This shows the I_2 estimate, which proves claim (38).

7. Another superposition. Specializing to $\rho(x) = (x - y) \cdot \nu$, one can also take the superposition with respect to ν. We will carry this out for $d = 3$. Starting with an inversion formula for the Radon transform,

$$
f(x) = -\frac{1}{8\pi^2} \Delta \left(\int_{S^2} d\nu \left(\int_{(x-y) \cdot \nu = 0} f(y) dA_y \right) \right),
$$

and noting that $\int_{S^2} d\nu \int_{(x-y) \cdot \nu = 0} f(y) dA_y$ tends to zero as $|x| \to \infty$ when $f \in C_c(\mathbb{R}^3)$, it follows that

$$
\int_{S^2} d\nu \left(\int_{(x-y) \cdot \nu = 0} f(y) dA_y \right) = 2\pi \int_{\mathbb{R}^3} \frac{f(y)}{|x - y|} dy.
$$

In other words, we have

$$
\int_{S^2} \delta(x \cdot \nu) d\nu = \frac{2\pi}{|x|}
$$

as a distribution. Hence, ignoring ρ and the lower order term

$$
\int_{S^2} g(\nu, y, k) d\nu = \frac{2\pi i}{k} \frac{e^{-k|x-y|^2}}{|x - y|} =_{def} h(x; y, k),
$$

we have that $\int_{S^2} u_{GB}(x; \nu, y)d\nu$ is an approximation to the outgoing solution to $L_n u = h$ satisfying the estimate (22).

Appendix. Form of the Green's function. Let $G_\lambda(x)$ be the free space Green's function for the Helmholtz equation at complex-valued wave number $\lambda = |\lambda|\beta$, where β is a complex number with $|\beta| = 1$ and $\Im\beta \geq 0$. The Green's function has the following properties:

(45) $\quad G_\lambda(x) = O(e^{-\Im\lambda|x|}|x|^{\frac{1-d}{2}}), \quad \partial_r G_\lambda(x) - i\lambda G_\lambda(x) = O(|x|^{\frac{1-d}{2}}), \quad r = |x| \to \infty.$

The dependence on $|\lambda|$ can be scaled out, and by rotational invariance we can write $G_\lambda(x) = |\lambda|^{d-2}\bar{G}_\beta(|\lambda x|)$, where $G_\beta(x) = \bar{G}_\beta(|x|)$. Then, if

$$\bar{G}_\beta(r) = \frac{e^{i\beta r}}{(\beta r)^{\frac{d-1}{2}}}\bar{w}_\beta(r),$$

the complex-valued function $\bar{w}_\beta$ will satisfy the following ODE for $r > 0$:

(46) $\quad \bar{w}_\beta''(r) + 2i\beta\bar{w}_\beta'(r) - \frac{c_d}{r^2}\bar{w}_\beta(r) = 0, \qquad c_d = \left(\frac{d-2}{2}\right)^2 - \frac{1}{4}.$

This we obtain by applying the Helmholtz operator in d dimensions to G_β away from $x = 0$ (with $r = |x|$) as follows:

$$0 = \Delta G_\beta(x) + \beta^2 G_\beta(x) = \frac{d^2}{dr^2}\bar{G}_\beta(r) + \frac{d-1}{r}\frac{d}{dr}\bar{G}_\beta(r) + \beta^2\bar{G}_\beta(r)$$

$$= \frac{e^{i\beta r}}{(\beta r)^{\frac{d-1}{2}}}\left(\bar{w}_\beta''(r) + 2i\beta\bar{w}_\beta'(r) - \frac{(d-1)(d-3)}{4}\frac{\bar{w}_\beta(r)}{r^2}\right).$$

After differentiating (46) p times we get

(47) $\quad \bar{w}_\beta^{(p+2)}(r) + 2i\beta\bar{w}_\beta^{(p+1)}(r) + \sum_{j=0}^{p} d_{p,j}\bar{w}_\beta^{(j)}(r)r^{-2-p+j} = 0$

for some coefficients $d_{p,j}$. From the left property in (45) it follows that $|\bar{w}_\beta(r)| \leq B_0$ for some bound B_0 and $r > 1$. Moreover, the right property (the radiation condition) implies that $\bar{w}_\beta' \to (d-1)\bar{w}_\beta/2r$ as $r \to \infty$. It then follows by induction on (47) that $\bar{w}_\beta^{(p)}(r) \to 0$ for all $p \geq 1$.

We now claim that there are bounds B_p, independent of r, such that $|r^p\bar{w}_\beta^{(p)}(r)| \leq B_p$ for $r > 1$. We just saw that this is true for $p = 0$, and we make the induction hypothesis that it is true for $j = 0, \ldots, p$. Then from (47),

$$\left|\frac{d}{dr}e^{2i\beta r}\bar{w}_\beta^{(p+1)}(r)\right| = e^{-2r\Im\beta}\left|\bar{w}_\beta^{(p+2)}(r) + 2i\beta\bar{w}_\beta^{(p+1)(r)}\right|$$

$$\leq e^{-2r\Im\beta}\sum_{j=0}^{p}|d_{p,j}||\bar{w}_\beta^{(j)}(r)|r^{-2-p+j} \leq B_{p+1}'e^{-2r\Im\beta}r^{-2-p},$$

when $r > 1$, where $B_{p+1}' = \sum_{j=0}^{p}|d_{p,j}B_j|$. Since $\bar{w}_\beta^{(p+1)}(r) \to 0$ as $r \to \infty$ and $\Im\beta \geq 0$,

$$\left|\bar{w}_\beta^{(p+1)}(r)\right| = e^{2r\Im\beta}\left|\int_r^\infty \frac{d}{ds}e^{2i\beta s}\bar{w}_\beta^{(p+1)}(s)ds\right| \leq B_{p+1}'\int_r^\infty \frac{e^{2(r-s)\Im\beta}}{s^{p+2}}ds$$

$$\leq \int_r^\infty \frac{B_{p+1}'}{s^{p+2}}ds = \frac{B_{p+1}}{r^{p+1}},$$

where $B_{p+1} = B'_{p+1}/(p+1)$. This shows the claim.

We conclude that

$$G_\lambda(x) = |\lambda|^{d-2} \bar{G}_\beta(|\lambda x|) = \frac{e^{i\lambda|x|}}{|x|^{\frac{d-1}{2}}} w(x; \lambda), \qquad w(x; \lambda) = |\lambda|^{\frac{d-3}{2}} \beta^{\frac{1-d}{2}} \bar{w}_\beta(|\lambda x|),$$

and for any multi-index α,

$$|\partial_x^\alpha w(x; \lambda)| \le C|\lambda|^{\frac{d-3}{2}} \sum_{j=0}^{|\alpha|} \left| \frac{d^j}{dr^j} \bar{w}_\beta(|\lambda r|) \right|_{r=|x|} = |\lambda|^{\frac{d-3}{2}} \sum_{j=0}^{|\alpha|} \left| \lambda^j \bar{w}_\beta^{(j)}(\lambda|x|) \right|$$

$$= |\lambda|^{\frac{d-3}{2}} \sum_{j=0}^{|\alpha|} B_j |x|^{-j} \le C(\delta)|\lambda|^{\frac{d-3}{2}},$$

when $|x| > \delta$ and $|\lambda| > 1/\delta$.

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