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Reflectionless Boundary Propagation Formulas for Partial Wave Solutions to the Wave Equation *

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Abstract

We consider solutions to the wave equation in 3+1 spacetime dimensions whose data is compactly supported at some initial time. For points outside a ball containing the initial support, we develop an outgoing wave condition, and associated one-way propagation formula, for the partial waves in the spherical-harmonic decomposition of the solution. The propagation formula expresses the l-th partial wave at time t and radius a in terms of order-l radial derivatives of the partial wave at time $t - \Delta t$ and radius $a - \Delta t$. The boundary propagation formula can be applied to any differential equation that is well-approximated by the wave equation outside a fixed ball.

1 Introduction

For hyperbolic partial differential equations with analytic coefficients, Warchall [3-4] established the local domain of dependence for solutions that, intuitively speaking, consist of waves that are outgoing outside a convex region. Analytic continuation was employed to establish those results, leaving open the question of whether there are explicit one-sided propagation formulas that serve to advance solutions in time in spatial regions where waves are outgoing. To date, the only explicit example of such a propagation formula has been that in [3] for the wave equation in one spatial dimension. Here we provide another example, for the wave equation in three spatial dimensions.

For the wave equation $\frac{\partial^2 u}{\partial t^2} - \Delta u = f$ in 3+1 spacetime dimensions, the results in [3] imply the following. Suppose that for all times t the source f (which could depend on u) has spatial support in the ball B of radius b centered, say, at the origin. Suppose $u(x, t)$ is a solution whose data at time t_0 is supported in B.

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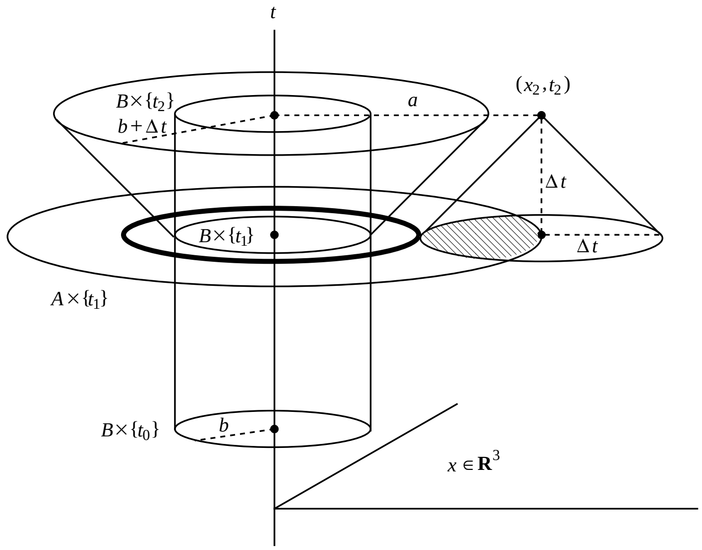

Figure 1: Spacetime Regions

Let $t_2 > t_1 > t_0$, and set $\Delta t \equiv t_2 - t_1$. Let $x_2 \in \mathbb{R}^3$ be such that $|x_2| > b + \Delta t$, and let A be the ball of radius $a \equiv |x_2|$ centered at the origin. Then $u(x_2, t_2)$ and $\frac{\partial u}{\partial t}(x_2, t_2)$ are completely determined by the data at time t_1 in the spatial region that is the intersection of A with the ball of radius Δt centered at x_2. This region is shown by the shaded area in the schematic Figure 1.

In this paper, we do not quite achieve the goal of making this dependence explicit. Instead, we exhibit an l-dependent one-sided propagation formula for the l-th partial wave in the spherical harmonic decomposition of u outside of B. This results in a formula for $u(x_2, t_2)$ in terms of (radial derivatives of) the data on the sphere of radius $|x_2| - \Delta t$ at the time t_1. While this formula is local in the radial coordinate, it involves data on an entire sphere surrounding B, shown as a heavy circle in Figure 1. Still open is the problem of determining a formula for $u(x_2, t_2)$ in terms of data at time t_1 in the intersection of A with the ball of radius Δt centered at x_2.

Our construction begins with the idea of Grote and Keller ([2]) to expand u in spherical harmonics and to determine an operator that converts the partial waves into solutions of the wave equation in one spatial dimension. Our work differs from theirs in that we employ a differential operator instead of an integral operator, allowing us to obtain a single-point propagation formula, in addition to differential boundary conditions.

2 Outgoing Wave Condition

Suppose u is a classical solution to the homogeneous wave equation in 3+1 spacetime dimensions. Let (r, θ, ϕ) be spherical coordinates for $\mathbb{R}^3$. Let

$$Y_{lm}(\theta, \phi) = \sqrt{\frac{(2l+1)(l-m)!}{4\pi(l+m)!}} P_l^m(\cos\theta) e^{im\phi}$$

be the normalized spherical harmonic function, where

$$P_l^m(z) = \frac{(-1)^m}{2^l l!}(1-z^2)^{m/2} \frac{d^{l+m}}{dz^{l+m}} \left[(z^2-1)^l\right]$$

is the associated Legendre function. We expand u in spherical harmonics: $u(x,t) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} u_{lm}(x,t)$, where $u_{lm}(x,t) \equiv v_{lm}(r,t) Y_{lm}(\theta,\phi)$ and

$$v_{lm}(r,t) \equiv \int_0^{2\pi} \int_0^{\pi} \overline{Y_{lm}(\theta,\phi)}\, u(r,\theta,\phi,t) \ \sin\theta \ d\theta \ d\phi \ .$$

Then v_{lm} satisfies $\frac{\partial^2 v_{lm}}{\partial t^2} = v_{lm}'' + \frac{2}{r} v_{lm}' - \frac{l(l+1)}{r^2} v_{lm}$, where a prime denotes partial differentiation with respect to r. We may transform this equation to remove one term by setting $y_{lm}(r,t) \equiv r^{-l} v_{lm}(r,t)$. Then y_{lm} satisfies $\frac{\partial^2 y_{lm}}{\partial t^2} = y_{lm}'' + \frac{2(l+1)}{r} y_{lm}'$. This is the Euler-Poisson-Darboux equation in odd spatial dimension, which may be transformed to the one-dimensional wave equation. Assuming y_{lm} is $(l+2)$ times continuously differentiable in r, we set $z_{lm}(r,t) \equiv \left(\frac{1}{r}\frac{\partial}{\partial r}\right)^l \left[r^{2l+1} y_{lm}(r,t)\right]$. Then, by virtue of the identity ([1])

$$\frac{\partial^2}{\partial r^2} \left(\frac{1}{r}\frac{\partial}{\partial r}\right)^{l-1} \left[r^{2l-1}\psi\right] = \left(\frac{1}{r}\frac{\partial}{\partial r}\right)^{l} \left[r^{2l}\frac{\partial \psi}{\partial r}\right] \tag{1}$$

for $\psi \in C^{l+1}$, the function z_{lm} satisfies $\frac{\partial^2 z_{lm}}{\partial t^2} = \frac{\partial^2 z_{lm}}{\partial r^2}$.

We denote with a dot partial differentiation with respect to time t. Under the hypothesis that both u and $\dot{u}$ have spatial support in the ball B at time t_0, it follows that the supports of $z_{lm}(\ \cdot, t_0)$ and $\dot{z}_{lm}(\ \cdot, t_0)$ are contained in $[0, b]$, since $z_{lm}(r,t) = \left(\frac{1}{r}\frac{\partial}{\partial r}\right)^l \left[r^{l+1} v_{lm}(r,t)\right]$. Because z_{lm} is a solution to the one-dimensional wave equation, it follows that, for all $t > t_0$ and $r > b$, $\frac{\partial z_{lm}}{\partial t}(r,t) + \frac{\partial z_{lm}}{\partial r}(r,t) = 0$. Consequently, v_{lm} satisfies the outgoing wave condition

$$\frac{\partial}{\partial r}\left(\frac{1}{r}\frac{\partial}{\partial r}\right)^l \left[r^{l+1} v_{lm}(r,t)\right] + \left(\frac{1}{r}\frac{\partial}{\partial r}\right)^l \left[r^{l+1}\frac{\partial v_{lm}}{\partial t}(r,t)\right] = 0 \tag{2}$$

for $t > t_0$ and $r > b$. This, evaluated at radius $r = a$, is the boundary condition of [2].

It is convenient to rewrite the outgoing wave condition (2) in a more compact form. Define the differential operator $L_l \equiv s^l \left(-\frac{\partial}{\partial s}\frac{1}{s}\right)^l$, and denote by L_l^* its formal adjoint $L_l^* \equiv \left(\frac{1}{s}\frac{\partial}{\partial s}\right)^l \left[s^l \cdot\right]$. With this notation, the outgoing wave condition for $v = v_{lm}(r,t)$ can be written as

$$\frac{\partial}{\partial s} L_l^* \left(s\, v\right) + L_l^* \left(s\, \dot{v}\right) = 0 \tag{3}$$

3 One-Sided Propagation Formula

We may use (3) to advance the solution u in time at locations with $r > b$ as follows. Each partial wave u_{lm} satisfies the (3+1)-dimensional wave equation, so we may apply the usual propagation formula to advance u_{lm} in time:

$$\begin{aligned} 4\pi u_{lm}(x,t_2) = \oint \{ \quad & u_{lm}(x+(\Delta t)\omega, t_1) + (\Delta t)\left[\dot{u}_{lm}(x+(\Delta t)\omega, t_1) + \right. \\ & \left. + (\omega\cdot\nabla u_{lm})(x+(\Delta t)\omega, t_1)\right] \}\, d^2\omega, \end{aligned}$$

where the integration is over the unit sphere.

Consider a location x_2 with $|x_2| > b + \Delta t$, and set $a \equiv |x_2|$. We will temporarily assume that the direction of x_2 is along the north pole of the spherical coordinate system. Because $Y_{lm}(\theta = 0, \phi) = 0$ for $m \neq 0$, we see that, with this assumption, $u_{lm}(x_2, t) = 0$ for $m \neq 0$, for all t. Thus $u(x_2,t) = \sum_{l=0}^{\infty} u_{l0}(x_2,t)$, and we consider only the time development of

$$u_{l0}(x,t) = \sqrt{\tfrac{2l+1}{4\pi}} P_l(\cos\theta) v_{l0}(r,t),$$

where P_l is the lth-order Legendre polynomial.

Substituting $w_l(x,t) \equiv \sqrt{\frac{4\pi}{2l+1}} u_{l0}(x,t) = v_{l0}(r,t) P_l(\cos\theta)$ into the propagation formula, changing to integration variable $s \equiv \frac{1}{a}\left|x_2 + (\Delta t)\omega\right|$, and integrating by parts the term involving $\frac{\partial}{\partial r} v_{l0}$, we arrive at the formula

$$2w_l(x_2,t_2) = \frac{s(s-\mu)}{\tau} P_l(\mu)\, v(s)\, \Big|_{s=1-\tau}^{s=1+\tau} + \int_{1-\tau}^{1+\tau} \left\{ sP_l(\mu)\dot{v}(s) - \tau\, P_l'(\mu) v(s) \right\}\, ds, \tag{4}$$

where for brevity we set $\mu \equiv \mu(s) \equiv \frac{s^2+1-\tau^2}{2s}$ and $\tau \equiv \frac{\Delta t}{a}$ and $v(s) \equiv v_{l0}(as,\ t_1)$ and $\dot{v}(s) \equiv a\, \frac{\partial v_{l0}}{\partial t}(as,\ t_1)$.

To make use of the outgoing wave condition (3), we will rewrite the term in (4) involving $\dot{v}$. We will manufacture the expression $L_l^*\left(s\, \dot{v}\right)$ from the term $sP_l(\mu)\dot{v}$ in the integrand of (4) by determining a function $Q_l(s)$ such that $P_l(\mu) = L_l(Q_l)$. Then integration by parts will convert the integrand term $sP_l(\mu)\dot{v} = L_l(Q_l)\ s\dot{v}$ to the term $Q_l\, L_l^*(s\dot{v})$, which according to the outgoing wave condition is equal to $-\,Q_l\, \frac{\partial}{\partial s} L_l^*(sv)$.

Additional integration by parts converts this term to $s\,v\,L_l\left(\frac{\partial}{\partial s}Q_l\right)$, which turns out to be equal to the opposite of the only other integrand term, $-\,\tau\,P_l'(\mu)v$, thus converting the integrand in (4) to zero and reducing the integral to boundary terms. We will furthermore choose our function $Q_l(s)$ such that all boundary terms at $s = 1+\tau$ vanish.

The required function $Q_l(s)$ could be obtained by direct l-fold integration of the criterion $P_l(\mu) = L_l(Q_l)$ with judicious choice of constants of integration. We prefer, however, to define $Q_l(s)$ as the result of that process.

Definition: For fixed τ and nonnegative integer l, we set

$$Q_l(s) \equiv \frac{(-1)^l}{2^l l!}\left((s-\tau)^2 - 1\right)^l .$$

In terms of the given definitions of L_l and μ, we have the following facts.

Lemma 1: $s\,L_l\left(\frac{\partial}{\partial s}Q_l\right) = \tau\,P_l'(\mu)$ for all nonnegative integer l.

Lemma 2: $L_l(Q_l) = P_l(\mu)$ for all nonnegative integer l.

Lemma 3: For integer $l \geq 1$ and functions f and g in $C^l(\mathbb{R})$,

$$\int_\alpha^\beta (L_l f)(s)\; g(s)\; ds = \Gamma_l(f,g)(s)\big|_{s=\alpha}^{s=\beta} + \int_\alpha^\beta f(s)\; (L_l^* g)(s)\; ds,$$

where

$$\Gamma_l(f,g)(s) \equiv -\sum_{j=1}^{l}\left[\left(-\frac{\partial}{\partial s}\frac{1}{s}\right)^{l-j} f(s)\right]\;\left[\frac{1}{s}\left(\frac{1}{s}\frac{\partial}{\partial s}\right)^{j-1}\left(s^l g(s)\right)\right].$$

The proofs of Lemma 1 and Lemma 2 are in Section 6. Lemma 3 is established by straightforward integration by parts.

We now use these results to carry out the computation outlined above for the term involving $\dot v$ in our integral formula (4):

For $l = 0$ we have

$$\int_{1-\tau}^{1+\tau} sP_0(\mu)\dot v(s)\,ds = \int_{1-\tau}^{1+\tau} s\,\dot v(s)\,ds = -\int_{1-\tau}^{1+\tau}\frac{\partial}{\partial s}(\,s\,v)\,ds$$

from direct application of the outgoing wave condition. Since $P_0'(z) = 0$ for all z, formula (4) reduces in this case to $2w_0(x_2,t_2) = \frac{s(s-\mu-\tau)}{\tau}v(s)\Big|_{s=1-\tau}^{s=1+\tau}$. Since $\mu(1+\tau) = \mu(1-\tau) = 1$, we have $w_0(x_2,t_2) = (1-\tau)\;v(1-\tau)$.

For $l \geq 1$ we have

$$
\begin{aligned}
&\int_{1-\tau}^{1+\tau} sP_l(\mu)\dot{v}(s)\,ds \\
&= \int_{1-\tau}^{1+\tau} L_l(Q_l)\, s\,\dot{v}(s)\,ds \qquad \text{(by Lemma 2)} \\
&= \Gamma_l(Q_l,\, s\dot{v})\big|_{1-\tau}^{1+\tau} + \int_{1-\tau}^{1+\tau} Q_l(s)\ L_l^*\,(s\,\dot{v})\ ds \qquad \text{(by Lemma 3)} \\
&= \Gamma_l(Q_l,\, s\dot{v})\big|_{1-\tau}^{1+\tau} + \int_{1-\tau}^{1+\tau} Q_l(s)\ \left(-\frac{\partial}{\partial s}L_l^*\,(s\,v)\right)\ ds \qquad \text{(by (3))} \\
&= [\Gamma_l(Q_l,\, s\dot{v}) - Q_l(s)L_l^*\,(s\,v)\,]\big|_{1-\tau}^{1+\tau} + \\
&\quad + \int_{1-\tau}^{1+\tau} \left(\frac{\partial}{\partial s}Q_l(s)\right)\ L_l^*\,(s\,v)\ ds \qquad \text{(by I.B.P)} \\
&= \big[\Gamma_l(Q_l,\, s\dot{v}) - \Gamma_l(\tfrac{\partial}{\partial s}Q_l,\, sv) - Q_l(s)L_l^*\,(s\,v)\,\big]\big|_{1-\tau}^{1+\tau} + \\
&\quad + \int_{1-\tau}^{1+\tau} L_l\left(\tfrac{\partial}{\partial s}Q_l\right)\ s\,v(s)\ ds \qquad \text{(by Lemma 3)} \\
&= \big[\Gamma_l(Q_l,\, s\dot{v}) - \Gamma_l(\tfrac{\partial}{\partial s}Q_l,\, sv) - Q_l(s)L_l^*\,(s\,v)\,\big]\big|_{1-\tau}^{1+\tau} + \\
&\quad + \int_{1-\tau}^{1+\tau} \tau\,P_l'(\mu)\,v(s)\ ds. \qquad \text{(by Lemma 1)}
\end{aligned}
$$

Thus our integral formula for the solution becomes

$$
\begin{aligned}
2w_l(x_2,t_2) \quad = \quad & \big[\tfrac{1}{\tau}s(s-\mu)P_l(\mu)\,v(s) + \Gamma_l(Q_l,\, s\dot{v}) \\
& -\ \Gamma_l(\tfrac{\partial}{\partial s}Q_l,\, sv) - Q_l(s)L_l^*\,(s\,v)\,\big]\big|_{s=1-\tau}^{s=1+\tau}
\end{aligned}
\tag{5}
$$

We claim that the expression in square brackets in (5) vanishes for $s = 1+\tau$. The reasons are the following.

For $l \geq 1$, it follows immediately from the definition of Q_l that $Q_l(1+\tau) = 0$. Thus the last term $-Q_l(s)L_l^*\,(s\,v)$ vanishes for $s = 1+\tau$. It also follows from the definition that derivatives of $Q_l(s)$ of orders less than l vanish at $s = 1+\tau$, because every such derivative contains at least one factor of $\big((s-\tau)^2 - 1\big)$. Because the quantity $\Gamma_l(f,g)$ involves derivatives of f and g only of orders $0,\ 1,\ \ldots,\ (l-1)$, the term $\Gamma_l(Q_l,\, s\dot{v})$ vanishes for $s = 1+\tau$.

In contrast, the summation in the third term $-\Gamma_l(\frac{\partial}{\partial s}Q_l,\, sv)$ contains exactly one term with an order-l derivative of Q_l. To evaluate this term at $s = 1+\tau$, let V.T. stand for terms that are polynomial in s and contain at least one factor of $\big((s-\tau)^2 - 1\big)$; such terms vanish when evaluated with $s = 1+\tau$. Bearing in mind that derivatives of $Q_l(s)$ of orders less than l vanish at $s = 1+\tau$, for the third term in (5) we have

$$\begin{aligned}
-\Gamma_l(\tfrac{\partial}{\partial s}Q_l,\, sv) &= \sum_{j=1}^{l}\left[\left(-\frac{\partial}{\partial s}\frac{1}{s}\right)^{l-j}\tfrac{\partial}{\partial s}Q_l\right]\left[\frac{1}{s}\left(\frac{1}{s}\frac{\partial}{\partial s}\right)^{j-1}\left(s^l sv\right)\right]\\
&= \left[\left(-\frac{\partial}{\partial s}\frac{1}{s}\right)^{l-1}\tfrac{\partial}{\partial s}Q_l\right]\left[s^l v\right] + \text{V.T.}\\
&= -sv(-1)^l\tfrac{\partial^l}{\partial s^l}Q_l + \text{V.T.}\\
&= -sv\tfrac{1}{2^l l!}\tfrac{\partial^l}{\partial s^l}\left((s-\tau)^2-1\right)^l + \text{V.T.}\\
&= -sv(s-\tau)^l + \text{V.T.}
\end{aligned}$$

Thus

$$-\Gamma_l(\tfrac{\partial}{\partial s}Q_l,\, sv)\big|_{s=1+\tau} = -(1+\tau)\; v(1+\tau).$$

On the other hand, because $\mu(1+\tau)=1$ and $P_l(1)=0$ for all l, the first term in (5) yields $\frac{1}{\tau}s(s-\mu)P_l(\mu)\,v(s)\big|_{s=1+\tau} = (1+\tau)\,v(1+\tau)$, which cancels the contribution from the third term.

Since $\mu(1-\tau)=1$, our propagation formula becomes finally

$$\begin{aligned}
2w_l(x_2,t_2) = \;& (1-\tau)\,v(1-\tau) + \\
&+\left(Q_l(s)L_l^*\,(s\,v) + \Gamma_l(\tfrac{\partial}{\partial s}Q_l,\, sv) - \Gamma_l(Q_l,\, s\dot{v})\right)\big|_{s=1-\tau}\,,
\end{aligned} \tag{6}$$

where $\tau \equiv \frac{\Delta t}{a}$ and $v(s) \equiv v_{l0}(as,\ t_1)$ and $\dot{v}(s) \equiv a\,\frac{\partial v_{l0}}{\partial t}(as,\ t_1)$. This formula expresses the value of $w_l(x_2,t_2)$ in terms of derivatives of v_{l0} at the single point $(r,t)=(a-\Delta t,\ t_1)$. Specifically, radial derivatives of $v_{l0}(r,\ t_1)$ to order l and of $\dot{v}_{l0}(r,\ t_1)$ to order $(l-1)$ are required, only at $r=a-\Delta t$. We note that formula (6) is also valid for $l=0$, provided $\Gamma_0(f,g)$ is defined to be zero.

4 Propagation at General Locations

We know how to advance $u(x_2,t)$ in time, using the one-sided propagation formulas for $w_l(x_2,t)=\sqrt{\frac{4\pi}{2l+1}}\;u_{l0}(x_2,t)$, in the case when the direction of x_2 is along the north pole ($\theta=0$) of the spherical coordinate system (r,θ,ϕ). For other directions of x_2 with, say, $(\theta,\phi)=(\theta_1,\phi_1)$, we may rotate the coordinate system to place x_2 along the new polar axis, compute the coefficients $v_{lm}^{(1)}(r,t)$ in the expansion of u with respect to spherical harmonics in the new coordinate system, and apply our propagation formula (6) to $v_{l0}^{(1)}(r,t)$ in place of $v_{l0}(r,t)$ to determine $w_l^{(1)}(x_2,t_2)$, and hence determine $u(x_2,t_2)=\sum_{l=0}^{\infty}\sqrt{\frac{2l+1}{4\pi}}\;w_l^{(1)}(x_2,t_2)$.

If we envisioned a numerical algorithm based on a truncated spherical-harmonic expansion combined with these results, we would find the recomputation of coefficients for different orientations of coordinate system to be wasteful.

Such recomputation is in fact unnecessary, because the coefficients are related by the addition formula for spherical harmonics:

$$\begin{aligned} v_{l0}^{(1)}(r,t) &= \sqrt{\frac{2l+1}{4\pi}} \int_0^{2\pi} \int_0^{\pi} P_l(\cos\theta')\ u(r,\theta,\phi,t)\ \sin\theta\ d\theta\ d\phi \\ &= \sqrt{\frac{4\pi}{2l+1}} \int_0^{2\pi} \int_0^{\pi} \sum_{m=-l}^{l} Y_{lm}(\theta_1,\phi_1)\, \overline{Y_{lm}(\theta,\phi)}\, u(r,\theta,\phi,t) \sin\theta\, d\theta\, d\phi \\ &= \sqrt{\frac{4\pi}{2l+1}} \sum_{m=-l}^{l} Y_{lm}(\theta_1,\phi_1)\ v_{lm}(r,t) \end{aligned}$$

This gives the coefficients $v_{l0}^{(1)}(r,t)$ in terms of the coefficients $v_{lm}(r,t)$ that can be computed once and for all in a fixed coordinate system.

We now insert this last expression for $v_{l0}^{(1)}$ into (6) to compute $w_l^{(1)}(x_2,t_2)$. Because (6) is linear in v and $\dot{v}$, and involves only radial derivatives, we may rearrange the sums to obtain

$$\begin{aligned} 2w_l^{(1)}(x_2,t_2) &= \sqrt{\tfrac{4\pi}{2l+1}} \sum_{m=-l}^{l} Y_{lm}(\theta_1,\phi_1) \Big[(1-\tau)\, v(1-\tau) + \\ &\quad + \left(Q_l(s) L_l^*\,(s\,v) + \Gamma_l(\tfrac{\partial}{\partial s} Q_l,\ sv) - \Gamma_l(Q_l,\ s\dot{v}) \right)\Big|_{s=1-\tau} \Big] \end{aligned}$$

where now $v(s) \equiv v_{lm}(as,\ t_1)$ and $\dot{v}(s) \equiv a\, \frac{\partial v_{lm}}{\partial t}(as,\ t_1)$.

Thus, for general $x_2 = (a,\theta_1,\phi_1)$, we have

$$u(x_2,t_2) = \sum_{l=0}^{\infty} \sqrt{\tfrac{2l+1}{4\pi}}\ w_l^{(1)}(x_2,t_2) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} Y_{lm}(\theta_1,\phi_1) v_{lm}(a,t_2)$$

where $v_{lm}(a,t_2)$ is obtained from the explicit one-sided propagation formula

$$\begin{aligned} v_{lm}(a,t_2) &= \tfrac{1}{2}(1-\tau)\, v(1-\tau) + \\ &\quad + \tfrac{1}{2}\left(Q_l(s) L_l^*\,(s\,v) + \Gamma_l(\tfrac{\partial}{\partial s} Q_l,\ sv) - \Gamma_l(Q_l,\ s\dot{v}) \right)\Big|_{s=1-\tau} \end{aligned} \tag{7}$$

where $\tau \equiv \frac{\Delta t}{a}$ and $v(s) \equiv v_{lm}(as,\ t_1)$ and $\dot{v}(s) \equiv a\, \frac{\partial v_{lm}}{\partial t}(as,\ t_1)$.

We note that, because $\frac{\partial u}{\partial t}(x,t)$ also satisfies the wave equation, we may obtain analogous propagation formulas for $\frac{\partial v_{lm}}{\partial t}(a,t_2)$ by applying (7) with $v(s)$ on the right-hand side replaced by $\frac{\partial v_{lm}}{\partial t}(as,t_1)$, and with $\dot{v}(s)$ on the right-hand side replaced by

$$a\frac{\partial^2 v_{lm}}{\partial t^2}(as,t_1) = a v_{lm}''(as,t_1) + \frac{2}{s} v_{lm}'(as,t_1) - \frac{l(l+1)}{as^2} v_{lm}(as,t_1).$$

In detail, our algorithm for advancing u on the boundary sphere $|x| = a > b + \Delta t$ from time t_1 to time $t_2 = t_1 + \Delta t$ is the following:

(I) Given initial data $u(x,t_1)$ and $\dot{u}(x,t_1)$ in a spatial neighborhood of the sphere of radius $(a-\Delta t)$, compute
$v_{lm}(r,t_1) \equiv \int_0^{2\pi}\int_0^{\pi} \overline{Y_{lm}(\theta,\phi)}\, u(r,\theta,\phi,t_1)\, \sin\theta\; d\theta\, d\phi$ and
$\dot{v}_{lm}(r,t_1) \equiv \int_0^{2\pi}\int_0^{\pi} \overline{Y_{lm}(\theta,\phi)}\, \dot{u}(r,\theta,\phi,t_1)\, \sin\theta\; d\theta\, d\phi$ for r near $(a-\Delta t)$, for $0 \le l \le N$ and $-l \le m \le l$, where N is the highest order of spherical harmonic to be used.

(II) Tabulate the numbers
$v_{lm}(a-\Delta t,t_1)$, $v'_{lm}(a-\Delta t,t_1)$, $v''_{lm}(a-\Delta t,t_1)$, . . . , $v^{(N+1)}_{lm}(a-\Delta t,t_1)$,
$\dot{v}_{lm}(a-\Delta t,t_1)$, $\dot{v}'_{lm}(a-\Delta t,t_1)$, $\dot{v}''_{lm}(a-\Delta t,t_1)$, . . . , $\dot{v}^{(N)}_{lm}(a-\Delta t,t_1)$,
for $0 \le l \le N$ and $-l \le m \le l$.

(III) Apply formula (7) to compute $v_{lm}(a,t_2)$ for $0 \le l \le N$ and $-l \le m \le l$. Apply the indicated modification of (7) to compute $\dot{v}_{lm}(a,t_2)$. Then $u(a,\theta,\phi,t_2) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} Y_{lm}(\theta,\phi)\; v_{lm}(a,t_2)$, with an analogous formula for $\dot{u}$ in terms of $\dot{v}_{lm}$.

(IV) Use these values for u and $\dot{u}$ on the boundary sphere $|x| = a$ together with the numerical algorithm of choice to update u and $\dot{u}$ for $|x| < a$.

(V) Repeat for the next time step. Note that the determination of $v_{lm}(a,t_2)$ is based on (spatial) derivatives of $v_{lm}(r,t_1)$ and $\dot{v}_{lm}(r,t_1)$ on the sphere $r = a-\Delta t$, which is inside the computational domain boundary. It is therefore conceivable that a numerical routine for the interior time development could be devised to maintain sufficient accuracy to allow accurate approximation of these radial derivatives.

5 Formulas for Low Values of l

The explicit terms in propagation formula (7) for cases $l = 0$ through $l = 4$ are given below.

$$v_{00}(a,t_2) = (1-\tau)\; v_{00}(a-\Delta t,\; t_1)$$

$$\begin{aligned} v_{1m}(a,t_2) \;&=\; (1-\tau)\;\; \{(1+\tau)v_{1m}(a-\Delta t,\; t_1)+ \\ &\quad +(1-\tau)(\Delta t)\,[\dot{v}_{1m}(a-\Delta t,\; t_1) + v'_{1m}(a-\Delta t,\; t_1)]\} \end{aligned}$$

$$\begin{aligned} v_{2m}(a,t_2) \;&=\; (1-\tau)^2\;\; \{(1+2\tau)v_{2m}(a-\Delta t,\; t_1)+ \\ &\quad +(\Delta t)\,[(1+2\tau)\dot{v}_{2m}(a-\Delta t,\; t_1) + (1+3\tau)v'_{2m}(a-\Delta t,\; t_1)] + \\ &\quad +(1-\tau)(\Delta t)^2\,[\dot{v}'_{2m}(a-\Delta t,\; t_1) + v''_{2m}(a-\Delta t,\; t_1)]\} \end{aligned}$$

$$\begin{aligned} v_{3m}(x_2,t_2) &= (1-\tau)\left\{(1+\tau)(1-5\tau^2)v_{3m}+\right. \\ &\quad +(1-\tau)(\Delta t)\left[(1+\tau)^2\dot v_{3m}+(1+3\tau-\tau^2)v'_{3m}\right]+ \\ &\quad +(1-\tau)^2(\Delta t)^2\left[\tfrac{1}{3}(3+10\tau)\dot v'_{3m}+(1+4\tau)v''_{3m}\right]+ \\ &\quad \left.+\tfrac{2}{3}(1-\tau)^3(\Delta t)^3\left[\dot v''_{3m}+v'''_{3m}\right]\right\} \end{aligned}$$

$$\begin{aligned} & v_{4m}(a,t_2) \\ &\quad = (1-\tau)\left\{(1+\tau-9\tau^2-9\tau^3+6\tau^4)v_{4m}\ +\right. \\ &\qquad +(1-\tau)(\Delta t)\left[\tfrac{1}{3}(1-\tau)(3+9\tau+8\tau^2)\dot v_{4m}+(1+3\tau-5\tau^2-13\tau^3)v'_{4m}\right]+ \\ &\qquad +\tfrac{1}{3}(1-\tau)^2(\Delta t)^2\left[(3+10\tau+11\tau^2)\dot v'_{4m}+(3+12\tau+7\tau^2)v''_{4m}\right]+ \\ &\qquad +\tfrac{1}{3}(1-\tau)^3(\Delta t)^3\left[(2+9\tau)\dot v''_{4m}+2(1+5\tau)v'''_{4m}\right]+ \\ &\qquad \left.+\tfrac{1}{3}(1-\tau)^4(\Delta t)^4\left[\dot v'''_{4m}+v^{(4)}_{4m}\right]\right\} \end{aligned}$$

In the last two formulas, we have omitted the arguments for the functions v_{lm} and $\dot v_{lm}$; they are, as always, $(a-\Delta t,\ t_1)$.

6 Proofs of Differentiation Formulas

In this section, we prove the differentiation formulas asserted in Lemmas 1 and 2. For completeness, we include a proof of formula (1):

Claim:

$$\frac{\partial^2}{\partial r^2}\left(\frac{1}{r}\frac{\partial}{\partial r}\right)^{l-1}\left[r^{2l-1}\psi\right]=\left(\frac{1}{r}\frac{\partial}{\partial r}\right)^{l}\left[r^{2l}\frac{\partial\psi}{\partial r}\right] \text{ for } \psi\in C^{l+1} \text{ and } l\ge 1.$$

Proof: By induction on l. We easily check that the formula holds in case $l=1$. Let $k\ge 2$ and make the inductive hypothesis that the formula holds for values of l less than k. Let $\psi\in C^{k+1}$. The right-hand side with $l=k$ can be rewritten

$$\left(\frac{1}{r}\frac{\partial}{\partial r}\right)^{k}\left[r^{2k}\frac{\partial\psi}{\partial r}\right]=\left(\frac{1}{r}\frac{\partial}{\partial r}\right)^{k-1}\left[r^{2(k-1)}\frac{\partial}{\partial r}\left(r\frac{\partial\psi}{\partial r}+(2k-1)\psi\right)\right].$$

By the inductive hypothesis with $l=k-1$ applied to the function $\phi\equiv r\frac{\partial\psi}{\partial r}+(2k-1)\psi$ in C^k, we have

$$\begin{aligned} \left(\frac{1}{r}\frac{\partial}{\partial r}\right)^{k}\left[r^{2k}\frac{\partial\psi}{\partial r}\right] &= \left(\frac{1}{r}\frac{\partial}{\partial r}\right)^{k-1}\left[r^{2(k-1)}\frac{\partial\phi}{\partial r}\right] \\ &= \frac{\partial^2}{\partial r^2}\left(\frac{1}{r}\frac{\partial}{\partial r}\right)^{k-2}\left[r^{2k-3}\phi\right] \end{aligned}$$

$$
\begin{aligned}
&= \frac{\partial^2}{\partial r^2}\left(\frac{1}{r}\frac{\partial}{\partial r}\right)^{k-2}\left[r^{2k-3}\left(r\frac{\partial\psi}{\partial r}+(2k-1)\psi\right)\right] \\
&= \frac{\partial^2}{\partial r^2}\left(\frac{1}{r}\frac{\partial}{\partial r}\right)^{k-1}\left[r^{2k-1}\psi\right]r
\end{aligned}
$$

which establishes the claim.

Formula (1) can be rewritten as a useful commutator relation for our operator L_l:

Corollary: $L_l\left(s\frac{\partial}{\partial s}f\right) - s\frac{\partial}{\partial s}L_l(f) = l\,L_l(f)$ for $f \in C^{l+1}$ and $s \neq 0$.

Proof: In case $l = 0$, when L_l is the identity operator, the assertion is trivially true. For $l \geq 1$, we first rewrite formula (1) with r replaced by s as

$$
\frac{\partial}{\partial s}\left(\frac{\partial}{\partial s}\frac{1}{s}\right)^{l}\left[s^{2l}\psi\right] = \frac{1}{s}\left(\frac{\partial}{\partial s}\frac{1}{s}\right)^{l}\left[s\frac{\partial}{\partial s}\left(s^{2l}\psi\right) - 2l\,s^{2l}\psi\right].
$$

Using the definition of L_l and setting $\psi(s) \equiv \frac{1}{s^{2l}}f(s)$, we obtain

$$
\frac{\partial}{\partial s}\left[\frac{1}{s^l}L_l(f)\right] = \frac{1}{s^{l+1}}L_l\left(s\frac{\partial}{\partial s}f\right) - \frac{2l}{s^{l+1}}L_l(f).
$$

Carrying out the differentiation in the first term, we arrive at the formula asserted.

We now prove Lemmas 1 and 2 simultaneously.

Lemma 4: $L_l(Q_l) = P_l(\mu)$ and $s\,L_l\left(\frac{\partial}{\partial s}Q_l\right) = \tau\,P_l'(\mu)$ for $s \neq 0$, for all non-negative integer l.

Proof: We proceed by induction on l. The formulas $L_l(Q_l) = P_l(\mu)$ and $s\,L_l\left(\frac{\partial}{\partial s}Q_l\right) = \tau\,P_l'(\mu)$ are trivially true in case $l = 0$. Let $k \geq 1$ and make the inductive hypothesis that both formulas hold for values of l less than k.

We begin by establishing the validity of the formula $s\,L_k\left(\frac{\partial}{\partial s}Q_k\right) = \tau\,P_k'(\mu)$. We note first that $\frac{\partial}{\partial s}Q_k(s) = (\tau - s)Q_{k-1}(s)$ for all s. The left-hand side of the assertion can thus be rewritten:

$$
\begin{aligned}
s\,L_k\left(\frac{\partial}{\partial s}Q_k\right) &= \tau\,sL_k(Q_{k-1}) - sL_k(sQ_{k-1}) \\
&= \tau\,s^{k+1}\left(\frac{-\partial}{\partial s}\frac{1}{s}\right)\left[\frac{1}{s^{k-1}}L_{k-1}(Q_{k-1})\right] + s^2L_{k-1}\left(\frac{\partial}{\partial s}Q_{k-1}\right).
\end{aligned}
$$

We apply the inductive hypothesis to obtain

$$
s\,L_k\left(\frac{\partial}{\partial s}Q_k\right) = \tau\,s^{k+1}\left(\frac{-\partial}{\partial s}\frac{1}{s}\right)\left[\frac{1}{s^{k-1}}P_{k-1}(\mu)\right] + s\tau\,P_{k-1}'(\mu).
$$

Using the fact that $\frac{\partial\mu}{\partial s} = 1 - \frac{\mu}{s}$, we perform the remaining derivative on the right-hand side and find

$$s\,L_k\left(\frac{\partial}{\partial s}Q_k\right) = \tau\left\{kP_{k-1}(\mu) + \mu P'_{k-1}(\mu)\right\} = \tau\,P'_k(\mu)$$

as claimed, where the last equality follows from properties of the Legendre polynomials.

We next establish the validity of the formula $L_k(Q_k) = P_k(\mu)$. We note first that

$$\begin{aligned}(s-\tau)\frac{\partial}{\partial s}Q_k &= (s-\tau)(\tau-s)Q_{k-1}\\ &= \left(1-(s-\tau)^2\right)Q_{k-1} - Q_{k-1}\\ &= 2kQ_k - Q_{k-1}\end{aligned}$$

for all s. Thus

$$L_k\left(s\frac{\partial}{\partial s}Q_k\right) = \tau\,L_k\left(\frac{\partial}{\partial s}Q_k\right) + 2kL_k(Q_k) - L_k(Q_{k-1}).$$

On the other hand, the commutation relation gives us

$$L_k\left(s\frac{\partial}{\partial s}Q_k\right) = s\frac{\partial}{\partial s}\,L_k\left(Q_k\right) + kL_k(Q_k),$$

so we have

$$s\frac{\partial}{\partial s}\,L_k\left(Q_k\right) - kL_k(Q_k) = \tau\,L_k\left(\frac{\partial}{\partial s}Q_k\right) - L_k(Q_{k-1}).$$

Now, it is straightforward to verify that $L_l(f) = -\frac{\partial}{\partial s}L_{l-1}(f) + \frac{l}{s}L_{l-1}(f)$ for $f \in C^l$, $l \geq 1$. Applying this identity to the term $L_k(Q_{k-1})$, we find

$$s\frac{\partial}{\partial s}\,L_k\left(Q_k\right) - kL_k(Q_k) = \tau\,L_k\left(\frac{\partial}{\partial s}Q_k\right) + \frac{\partial}{\partial s}L_{k-1}(Q_{k-1}) - \frac{k}{s}L_{k-1}(Q_{k-1}).$$

For the first term on the right-hand side, we make use of the formula $s\,L_k\left(\frac{\partial}{\partial s}Q_k\right) = \tau\,P'_k(\mu)$ established above. For the last two terms, we apply the inductive hypothesis, and we arrive at

$$s\frac{\partial}{\partial s}\,L_k\left(Q_k\right) - kL_k(Q_k) = \frac{\tau^2}{s}\,P'_k(\mu) + \frac{\partial}{\partial s}\left(P_{k-1}(\mu)\right) - \frac{k}{s}P_{k-1}(\mu).$$

Making use of the Legendre polynomial identity that relates P'_k and P'_{k-1} to eliminate P'_{k-1}, we simplify the right-hand side to obtain

$$s\frac{\partial}{\partial s}\,L_k\left(Q_k\right) - kL_k(Q_k) = (s-\mu)\,P'_k(\mu) - kP_k(\mu).$$

This may be rewritten as $s^{k+1}\frac{\partial}{\partial s}\left(\frac{1}{s^k}L_k(Q_k)\right) = s^{k+1}\frac{\partial}{\partial s}\left(\frac{1}{s^k}P_k(\mu)\right)$, which implies $\frac{1}{s^k}L_k(Q_k) = \frac{1}{s^k}P_k(\mu) + C_k$ for some constant C_k.

We may finally determine the constant by evaluating the expressions at $s = 1+\tau$. We have $P_k(\mu(1+\tau)) = P_k(1) = 1$. Since derivatives of $Q_k(s)$ of orders less than k contain factors of $\left((s-\tau)^2 - 1\right)$, we see

$$L_k(Q_k)|_{s=1+\tau} = \left(-\frac{\partial}{\partial s}\right)^k \left[\frac{(-1)^k}{2^k k!}\left((s-\tau)^2-1\right)^k\right]\Bigg|_{s=1+\tau} = 1.$$

Thus $C_k = 0$. This completes the proof of Lemma 4.

Remark: The identity $L_l(Q_l) = P_l(\mu)$, more explicitly

$$P_l\left(\frac{s^2-\tau^2+1}{2s}\right) = \frac{1}{2^l l!}s^l\left(\frac{\partial}{\partial s}\frac{1}{s}\right)^l \left((s-\tau)^2-1\right)^l,$$

is reminiscent of Rodrigues identity $P_l(x) = \frac{1}{2^l l!}\left(\frac{\partial}{\partial x}\right)^l \left(x^2-1\right)^l$. We do not know if it can be obtained directly from Rodrigues identity.

Remark: Straightforward integration of $L_l(Q_l) = P_l(\mu)$ shows that

$$Q_l(s) = s\int_s^{1+\tau} s_1 \int_{s_1}^{1+\tau} s_2 \int_{s_2}^{1+\tau} \cdots\ s_{l-1}\int_{s_{l-1}}^{1+\tau} \frac{1}{s_l^l}P_l(\mu(s_l))\ ds_l \cdots ds_2\, ds_1,$$

which would be the most natural definition of $Q_l(s)$, based on our original requirements for $Q_l(s)$. We discovered the defining formula used here for $Q_l(s)$ by observing the pattern in the explicit formulas that resulted from computation of this integral for small values of l.

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