A GEOMETRIC-OPTICAL SERIES AND A WKB PARADOX*

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Abstract. We discuss a solution of the one-dimensional reduced wave equation with non-constant velocity. We show that, for sufficiently small total velocity variations, this solution is exact. Furthermore, it lends itself to (high-frequency) asymptotic analysis and to elementary numerical analysis in a natural way. For reflected waves, we show that asymptotically small reflection implies numerically small reflection, thus resolving a paradox of classical WKB theory.

I. Introduction. The purpose of this paper is twofold. First, we discuss an exact solution of the wave equation problem

$$d^2y/dx^2 + (\omega^2/c^2(x))y = 0 \qquad (0 \leq x < \infty); \tag{1a}$$

$$dy/dx + (i\omega/c(0))y = 2i\omega/c(0) \qquad (x = 0); \tag{1b}$$

$$dy/dx - (i\omega/c(\infty))y \to 0 \qquad (x \to \infty) \tag{1c}$$

which has been applied to a problem in inverse scattering [1, 2]. (Here it is assumed that all variables are dimensionless; in particular, ω represents dimensionless frequency and $|\omega| \gg 1$ refers to waves of high frequency or short wavelength. It is also assumed that $c(x)$ tends smoothly to the limiting values $c(0)$ and $c(\infty)$ as x tends to zero and infinity.) We obtain from the solution of (1) an asymptotic expansion in powers of two parameters, in contrast to the classical WKB expansion in powers of a single parameter. Second, we discuss the relationship of this expansion to the "WKB paradox" of Meyer [3, 4] and Mahony [5]. In these references, the problem (1) is replaced by the analogous problem on $\mathbb{R}$. Our reason for addressing the problem on $[0, \infty)$ is that, for applications such as inverse scattering, the phase of the wave must be known exactly, whereas solving on $(-\infty, \infty)$ determines the phase only up to an additive constant. Also, our results will be immediately applicable to the problem restated on $\mathbb{R}$ merely by ignoring the results concerning the phase.

The problem (1) is generally solved either exactly by integral equation methods, or asymptotically (for large values of ω) by the WKB expansion. To solve (1) exactly, the differential equation (1a) is usually recast by means of the Langer transformation

$$\tau = \int_0^x dx_1/c(x_1), \tag{2a}$$

$$u = [c(0)/c(x)]^{1/2}y. \tag{2b}$$

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With independent and dependent variables transformed, there results a time-independent Schrödinger equation, for which variation of parameters provides an integral equation to be solved iteratively. (Mahony has adopted this approach in his formulation of the WKB paradox.) This provides a series in inverse powers of ω which is at least asymptotically valid as $|\omega|$ tends to infinity and which is convergent given some restrictions on $c(x)$. The disadvantage of this method is that the terms in the series have no clear physical interpretation. The classical WKB expansion (see, for example Erdelyi [6], pp. 78–85) has the same shortcoming.

An alternative approach to the solution of (1) has been developed by Bremmer [7]. In contrast to the formal mathematical procedures of the Langer transformation or the WKB expansion, Bremmer's solution is based on simple properties of one-dimensional waves (continuity across velocity jumps) and simple limiting arguments. His result is a series whose nth term denotes that part of the wave which has undergone n reflections; i.e., n is the "order" of reflection. The physical meaning of his result is that comparatively large (global) velocity variations give reflected waves comparatively large in magnitude. Bremmer's expansion is somewhat surprising in that it is frequency-independent and yet its first term is identical to that of the formal WKB (high-frequency) series.

Here we shall discuss a solution of (1) described by Gray and Hagin [1, 2]. This solution, like those of Mahony and Bremmer, is an infinite series of integrals. Unlike that of Mahony, however, it is not the solution of an equivalent Schrödinger equation and is not a series containing powers of ω^{-1}. Also, in contrast to Bremmer's solution, it is not based on physical properties of waves; it is the result of a formal mathematical procedure. But we shall demonstrate its equivalence to Bremmer's series, thereby bridging the gap between the mathematical and physical nature of solutions of (1). This series can easily and accurately be estimated numerically, or an expansion in powers of ω^{-1} can be obtained by asymptotically evaluating the integrals in the series. Such a "WKB" series will contain two parameters, one expressing high frequency and the other expressing both small reflections and order of reflection.

Next, we shall show how this geometric-optical series resolves the WKB paradox which, stated briefly, is the following. For $|\omega| \gg 1$, asymptotic analysis of the solution of (1) predicts that if $c(x)$ is $C^{(n-1)}$ smooth but not $C^{(n)}$ smooth on $[0, \infty)$, the reflected wave at $x = 0$ is $O(\omega^{-n})$. In particular, if $c(x)$ is C^{∞} then, no matter how rapidly varying $c(x)$ is, the reflected wave at $x = 0$ is asymptotically zero; and the paradox lies in the last statement. This has been noted by both Mahony and Meyer, and both have noted, by considering the zeros and poles of $c(x)$ in the complex plane, that asymptotic smallness of the reflected wave does not imply numerical smallness. However, these results do not explicitly show the cause of a numerically large reflected wave—i.e., large reflections due to large variations of $c(x)$ on the real axis. This is due to the absence of an adequate measure of size of velocity variations in the WKB expansion, and underlines the incompleteness of existing WKB theory as modified by Mahony and Meyer. By contrast, as we shall show, the Bremmer expansion can be analyzed in both high-frequency and small-velocity-variation limits for suitably restricted $c(x)$, and this analysis will not require $c(x)$ to be an analytic function. In these limits, asymptotic smallness of the reflected wave will imply numerical smallness. In addition, the relationship between the decay rate (in ω^{-1}) of the asymptotic expansion and smoothness of $c(x)$ will be explicit.

II. Derivation and discussion of the geometric-optical series. The first step in Gray and Hagin's solution of (1) is to recast it in terms of the travel time (2a). (This is "half" a Langer transformation.) With this transformation, the differential equation (1a) becomes

$$d^2y/d\tau^2 + \omega^2 y = 2R(\tau)(dy/d\tau), \tag{3}$$

where

$$R(\tau) = (2c)^{-1}\, dc/d\tau = (d/d\tau) \ln c/2. \tag{4}$$

The function $R(\tau)$ has been called a "reflectivity function" (Foster [8]) for the reason that (for differentiable $c(\tau)$)

$$\lim_{\Delta\tau \to 0} R(\tau)\, \Delta\tau = \lim_{\Delta\tau \to 0} \frac{\Delta c/\Delta\tau}{2c + \Delta c}\, \Delta\tau = \lim_{\Delta\tau \to 0} \frac{\Delta c}{2c + \Delta c}$$

is the local differential reflection coefficient of the medium.

The second step is the solution of Eq. (3) with transformed boundary conditions corresponding to (1b, c) by variation of parameters:

$$y(\tau, \omega) = \exp(i\omega\tau) + (i\omega)^{-1} \int_0^\infty d\tau_1 R(\tau_1) y'(\tau_1, \omega) \exp(i\omega\,|\tau - \tau_1|). \tag{5}$$

The iterative solution of (5), with $y_0 = \exp(i\omega\tau)$ as the zeroth iterate, is

$$y(\tau, \omega) = \exp(i\omega\tau) + \sum_{n=1}^{\infty} I_n(\tau, \omega), \tag{6}$$

where I_n is the n-fold repeated integral

$$\begin{aligned} I_n(\tau, \omega) = \int_0^\infty d\tau_1 \cdots \int_0^\infty d\tau_n\, R(\tau_1) \cdots R(\tau_n) \operatorname{sgn}[(\tau_1 - \tau_2) \cdots (\tau_{n-1} - \tau_n)] \\ \cdot \exp[i\omega(|\tau - \tau_1| + \cdots + |\tau_{n-1} - \tau_n| + \tau_n)]. \end{aligned} \tag{7}$$

A sufficient condition that (6–7) satisfy (3) for all (τ, ω) is that

$$\int_0^\infty |R(\tau)|\, d\tau < 1. \tag{8}$$

That a restriction like (8) is also necessary can be seen from the fact that an oscillatory non-decaying $R(\tau)$ such as $\sin(\omega_0 \tau)$ for fixed ω_0 can "beat" against the oscillatory integral kernel, causing divergence of the integrals for certain values of ω.

With the bound (8) on $R(\tau)$ (small reflections), the series (6–7) presents an exact solution of (3), but it does not show explicitly how the medium changes the wave passing through it. In particular, the WKB amplitude $(c(\tau)/c(0))^{1/2}$ is not evident in (6). Moreover, the lack of the WKB amplitude presents an apparent discrepancy between (6–7) and the solution obtained by Bremmer, which can be written in the form

$$y(\tau, \omega) = \sum_{n=0}^{\infty} \tilde{I}_n(\tau, \omega) \tag{9}$$

with

$$\tilde{I}_0(\tau, \omega) = [c(\tau)/c(0)]^{1/2} \exp(i\omega\tau), \tag{10a}$$

$$\tilde{I}_{2n+1}(\tau, \omega) = [c(\tau)]^{1/2}\int_\tau^\infty d\tau_1[c(\tau_1)]^{-1/2} \cdot R(\tau_1)\tilde{I}_{2n}(\tau_1, \omega)\exp[i\omega(\tau_1 - \tau)], \tag{10b}$$

$$\tilde{I}_{2n}(\tau, \omega) = -[c(\tau)]^{1/2}\int_0^\tau d\tau_1[c(\tau_1)]^{-1/2} \cdot R(\tau_1)R(\tau_1)\tilde{I}_{2n-1}(\tau_1, \omega)\exp[i\omega(\tau - \tau_1)]. \tag{10c}$$

But we shall demonstrate the equivalence of (6–7) with (9–10) in the following argument.

First, we observe that in (7), I_n does not refer to a fixed number (e.g., n) of reflections. To show this, we express I_n as a sum of 2^n integrals determined by the sgn functions and the absolute values in the phase. For example,

$$I_1(\tau, \omega) = \exp(i\omega\tau)\int_0^\tau d\tau_1 R(\tau_1) + \exp(-i\omega\tau)\int_\tau^\infty d\tau_1 R(\tau_1)\exp(2i\omega\tau_1).$$

In the second term of I_1, the interpretation is that of a single reflection at each $\tau_1 > \tau$. This is because the wave, propagating with velocity $c(\tau)$, has been delayed by $2(\tau_1 - \tau)$ in its path through the medium from zero to the point $x = \int_0^\tau c(\tau')\,d\tau'$; that is, the wave has propagated from zero to $x = \int_0^\tau c(\tau')\,d\tau'$ to $x_1 = \int_0^{\tau_1} c(\tau')\,d\tau'$ then back to x. The first term of I_1 expresses no reflections. In general, I_n contains terms with various numbers of reflections: a single zero-reflection term, n 1-reflection terms, $\binom{n}{k}$ k-reflection terms for $k \le n$. This can be seen merely by expanding (7) into 2^n integrals as suggested above.

Using this observation, we next combine the 0-reflection terms from all the I_ns to obtain the WKB amplitude for the "direct" wave. From I_n, the 0-reflection term is

$$\exp(i\omega\tau)\int_0^\tau d\tau_1 R(\tau_1) \cdots \int_0^{\tau_{n-1}} d\tau_n R(\tau_n),$$

which can be evaluated by recalling that $R(\tau) = (d/d\tau)\ln c/2$. After n iterated integrations, the result is that the 0-reflection term from I_n is rewritten as

$$\exp(i\omega\tau)[\ln(c(\tau)/c(0))/2]^n/n!$$

Summing over all n,

$$\exp(i\omega\tau)\left\{1 + \sum_{n=1}^\infty [\ln(c(\tau)/c(0))/2]^n/n!\right\} = \exp(i\omega\tau)\exp\{\ln(c(\tau)/c(0))/2\} = (c(\tau)/c(0))^{1/2}\exp(i\omega\tau).$$

This is the desired result—that the direct wave (0 reflections) has the WKB amplitude.

We complete the argument by indicating how the $(k + 1)$-reflection terms can be obtained given an expression containing all the k-reflection terms, thus duplicating the result of Bremmer. For simplicity we shall compute only the singly reflected wave from the direct wave; the general recursion is much more tedious. As mentioned above, $I_n(\tau, \omega)$ contains n 1-reflection terms; for example, one of the 5 1-reflection terms in I_5 is

$$\exp(-i\omega\tau)\int_\tau^\infty d\tau_1 R\int_{\tau_1}^\infty d\tau_2(-R)\int_{\tau_2}^\infty d\tau_3(-R)\exp(2i\omega\tau_3)\int_0^{\tau_3} d\tau_4 R\int_0^{\tau_4} d\tau_5 R$$

$$= \exp(-i\omega\tau)\int_\tau^\infty d\tau_1 R\int_{\tau_1}^\infty d\tau_2(-R)\int_{\tau_2}^\infty d\tau_3(-R)\exp(2i\omega\tau_3)[\ln(c(\tau_3)/c(0))/2]^2/2!$$

By repeated partial integrations starting with τ_1, this can be shown to be equal to

$$\exp(-i\omega\tau)\int_\tau^\infty d\tau_1 R \exp(2i\omega\tau_1)[\ln(c(\tau)/c(\tau_1))/2]^2[\ln(c(\tau_1)/c(0))/2]^2/(2!\,2!)$$

In general for $n = r + s + 1$, I_{r+s+1} will contain $(r + s + 1)$ 1-reflection terms, each of the form

$$\exp(-i\omega\tau)\int_\tau^\infty d\tau_1 R(\tau_1)\exp(2i\omega\tau_1)[\ln(c(\tau)/c(\tau_1))/2]^r[\ln(c(\tau_1)/c(0))/2]^s/(r!\,s!).$$

Summing over all n gives the singly reflected wave:

$$\exp(-i\omega\tau)\sum_{r,s=0}^{\infty}\int_\tau^\infty d\tau_1 R(\tau_1)\exp(2i\omega\tau_1)[\ln(c(\tau)/c(\tau_1)/2]^r[\ln(c(\tau_1)/c(0))/2]^s/(r!\,s!)$$

$$= \exp(-i\omega\tau)\int_\tau^\infty d\tau_1 R(\tau_1)\exp(2i\omega\tau_1)[c(\tau)/c(\tau_1)]^{1/2}[c(\tau_1)/c(0)]^{1/2}$$

$$= [c(\tau)/c(0)]^{1/2}\exp(-i\omega\tau)\int_\tau^\infty d\tau_1 R(\tau_1)\exp(2i\omega\tau_1).$$

A similar computation shows that the expression for the part of the wavefield at $x = \int_0^\tau c(\tau_1)\,d\tau_1$ which has undergone two reflections is

$$-[c(\tau)/c(0)]^{1/2}\exp(i\omega\tau)\int_0^\tau d\tau_1 R \exp(-2i\omega\tau_1)\int_{\tau_1}^\infty d\tau_2 R \exp(2i\omega\tau_2).$$

If the nth reflected wave is written as $y_n(\tau, \omega)$, then the expression for the total wavefield which relates succeeding y_n's is

$$y(\tau, \omega) = \sum_{n=0}^{\infty} y_n(\tau, \omega) \tag{11}$$

with

$$y_0(\tau, \omega) = [c(\tau)/c(0)]^{1/2}\exp(i\omega\tau), \tag{12a}$$

$$y_{2n+1}(\tau, \omega) = [c(\tau)]^{1/2}\int_\tau^\infty d\tau_1 R(\tau_1)[c(\tau_1)]^{-1/2}\exp[i\omega(\tau_1 - \tau)]y_{2n}(\tau_1, \omega), \tag{12b}$$

$$y_{2n}(\tau, \omega) = -[c(\tau)]^{1/2}2\int_0^\tau d\tau_1 R(\tau_1)[c(\tau_1)]^{-1/2}\exp[i\omega(\tau - \tau_1)]y_{2n-1}(\tau_1, \omega). \tag{12c}$$

This expression agrees with (9–10), and shows that a rearrangement of the terms of the series (6–7) produces Bremmer's geometric-optical series.

The physical interpretation of, say, (12c) is straightforward. At a point τ, an ensemble of reflected arrivals from all points $\tau_1 < \tau$ occurs. Each of these arrivals has amplitude and phase given by $[c(\tau_1)]^{-1/2}y_{2n-1}(\tau_1, \omega)$ *before* being reflected forward to the point τ, and amplitude and phase of $-R(\tau_1)[(\tau_1)]^{-1/2}y_{2n-1}(\tau_1, \omega)$ immediately *after* the reflection at τ_1. The reason for the minus sign is that the local reflection coefficient of a left-traveling wave is the negative of that of a right-traveling wave. The phase factor $\exp[i\omega(\tau - \tau_1)]$ indicates the time of propagation from τ_1 to τ, and the factor $[c(\tau)]^{1/2}$ preserves amplitude as (WKB amplitude) $\times$ (effect of reflections).

III. Application of the geometric-optical series to the WKB paradox. To apply the results of the preceding section to the WKB paradox, we set $\tau = 0$ in (11–12) to obtain a series for the reflected wave whose terms express 1, 3, 5, $\cdots$ reflections. As mentioned earlier, this series will converge given sufficiently small $R(\tau)$, so that if

$$\int_0^\infty |R(\tau)|\,d\tau = O(\varepsilon) \quad \text{with} \quad \varepsilon \ll 1, \tag{13}$$

the series can be approximated by the sum of its first few terms. Thus for a moderately varying medium, the first few reflected waves are the most significant. (On the other hand, if $\int |R(\tau)|\,d\tau$ is not small because of oscillations in $R(\tau)$, much of the wave's energy will remain trapped in the medium for a long time. This is analogous to trapped modes in potential scattering.)

For the discussion of (11–12) with $\tau = 0$ we write

$$R(\tau) = \varepsilon \tilde{R}(\tau), \tag{14}$$

so that the series contains increasing powers of ε. It is evident that ε expresses small (total) reflections and that the power of ε refers to the number of reflections undergone by a particular term.

Now (11) can be evaluated by performing the integrals in (12). If these integrals are performed asymptotically, a WKB series in ω^{-1} and ε is the result; if numerically, a series in ε. We emphasize that the two parameters are independent of each other, and that each makes possible a fairly simple approximation evaluation of reflection. The high-frequency parameter ω^{-1} provides an expansion which is independent of reflection size $\int |R(\tau)|\,d\tau$, but which fails to give meaningful results if $c(x)$ is C^∞ smooth on $[0, \infty)$. The small-reflection parameter ε provides an expansion which is equally valid for all frequencies, is at least comparable to the WKB expansion if $c(x)$ has a discontinuous derivative, and is superior to the WKB expansion if $c(x)$ is C^∞ smooth (see Sec. IV). Also, the expansion in powers of ε eliminates the need to assume that $c(x)$ is analytic *near* the x-axis if smooth *on* the x-axis. The first reflection term

$$y_1(0, \omega) = \varepsilon \int_0^\infty d\tau_1 \tilde{R}(\tau_1) \exp(2i\omega\tau_1) \tag{15}$$

can be estimated either numerically by a discrete Fourier transform as in Sec. IV or asymptotically (for large $|\omega|$) by partial integration (Bleistein and Handelsman [9], Ch. 3). If, for simplicity, $R(\tau)$ is C^∞ smooth on $[0, \infty)$ except for a jump discontinuity of $R^{(N)}(\tau)$ at $\tau = c$, and $R(\tau)$ decays to zero as x tends to 0 and infinity, then, for $|\omega| \gg 1$,

$$y_1(0, \omega) \sim \varepsilon(-2i\omega)^{-N-1}[\tilde{R}^{(N)}(c_+) - \tilde{R}^{(N)}(c_-)]\exp(2i\omega c). \tag{16}$$

(This duplicates a result of Chester and Keller [10].) If $R(\tau)$ is C^∞ smooth on $[0, \infty)$, then $y_1(0, \omega) \sim 0$. The third reflection term,

$$y_3(0, \omega) = \varepsilon^3 \int_0^\infty d\tau_1 \tilde{R} \exp(2i\omega\tau_1) \int_0^{\tau_1} d\tau_2 \tilde{R} \exp(2i\omega\tau_2) \int_{\tau_2}^\infty d\tau_3 \tilde{R} \exp(2i\omega\tau_3), \tag{17}$$

can be analyzed similarly, beginning with the innermost integral. This term can be shown to be asymptotically smaller in ε and ω^{-1} than y_1. Higher reflection terms are of higher order in both ε and ω^{-1}.

These observations agree with those of Mahony and Meyer, namely, that a smoothly varying velocity admits a reflected wave asymptotically smaller than any power of ω^{-1}. The important differences, given (13), are: (i) "asymptotically small" here also means "numerically small"; (ii) based on the discussion of the next section, asymptotic smallness of the reflected wave does not impede its accurate evaluation. Thus, the condition (13) of small global velocity variations permits a resolution of the WKB paradox which directly relates size of the reflected wave with size of variations in velocity. This resolution also avoids reliance on "exponential asymptotics" which result from assuming that $c(x)$ is an analytic function near the real axis.

IV. An example. As a numerical illustration of the usefulness of (11–12) with $\tau = 0$, we consider reflections due to the velocity profile

$$\begin{aligned} c(x) &= 1 + \frac{\exp[-1/x]}{\exp[-1/x] + \exp[-1/(1-x)]} \quad , \quad 0 \le x \le 1 \\ &= 2 \quad , \quad x > 1 \end{aligned} \tag{18}$$

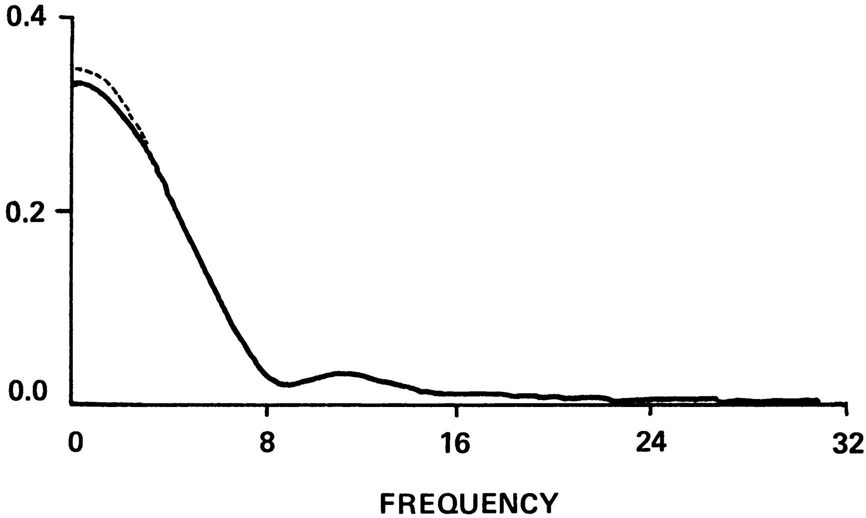
First, we note that $c(x)$ is C^∞ smooth so that classical WKB theory predicts zero reflection in the high frequency regime. Second, $c(x)$ is not analytic in a strip around the x-axis, so that exponential asymptotics cannot be applied. Third, $c(x)$ jumps from one to two between $x = 0$ and $x = 1$, and

$$\begin{aligned} \int_0^\infty |R(\tau)|\, d\tau &= \int_0^\infty (2c)^{-1} (dc/d\tau)\, d\tau = \int_0^1 (2c)^{-1} (dc/dx)\, dx \\ &= 2^{-1} \ln(c(1)/c(0)) \\ &= (\ln 2)/2 \approx 0.35, \end{aligned}$$

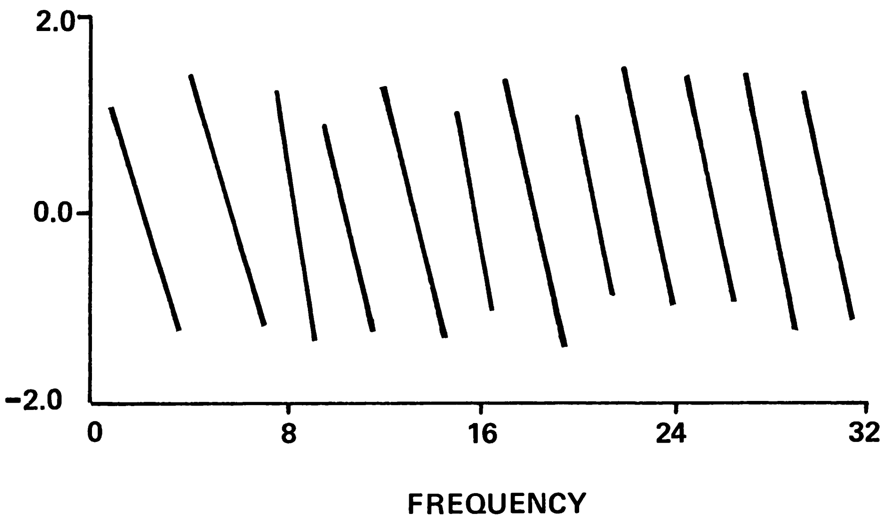
so that even a drastic change (doubling) of $c(x)$ produces $\int |R(\tau)|\, d\tau \ll 1$. For (18), we compared numerically the first reflection term (15) with the exact reflection response. Since it is not possible to obtain the exact reflection analytically (in fact, it is our objective here to determine a suitable approximation to the reflection), a numerical scheme (described in [11]) was used. Then, the integral (15) was calculated as follows. First, change variable from τ to x:

$$\int_0^\infty d\tau c^{-1}(dc/d\tau)\exp(2i\omega\tau) = \int_0^1 dx c^{-1}(dc/dx)\exp[2i\omega\tau(x)], \tag{19}$$

where we have used the fact that dc/dx has support in (0, 1). Next, compute $\tau(x)$ for each x in the mesh between 0 and 1 by using a Gaussian quadrature to evaluate (2a). Finally, for each desired ω, compute real and imaginary parts of the right-hand side of (19) by the trapezoid rule—the equivalent of a discrete Fourier transform. (The reason for the more accurate integration scheme in evaluating the numbers $\tau(x)$ is the need for high accuracy in the phase of (19), especially for large ω.) The comparison of exact vs. approximate reflection response appears in Fig. 1. It can be seen that numerical evaluation of (15) has yielded remarkable agreement with the exact reflection response for frequencies between 0.5 and 32. The greatest error in the magnitude was 4% at $\omega = .5$, and the plots of the phase are indistinguishable. Similar numerical experiments were either (13) is violated or $c(x)$ has a discontinuous derivative have yielded a similar result—excellent agreement between the



(a)



(b)

FIG. 1. Comparison of first term of the geometric-optical series with the exact reflection response. Exact response is solid curve; response computed from the geometric-optical series is dashed curve. (a) Magnitude; (b) Phase (two indistinguishable plots).

exact reflection response and the easily computed integral (15). (The integral (17) could, if necessary, be computed fairly easily as a correction term when (13) is violated.)

Finally, if the problem addressed in this paper had been stated on $(-\infty, \infty)$ rather than $[0, \infty)$, the only effect on this example would be to eliminate Fig. 1(b), since phase information on the reflected wave would be obtained only up to a phase shift.

V. Conclusions. We have discussed a solution of the one-dimensional reduced wave equation with variable coefficients; the solution appears in the form of an infinite series of integrals each term of which has a clear physical interpretation. By evaluating this series at a particular point, we obtained an expression for reflected plane waves. This expression was shown to be exact if the total reflectivity of the medium is sufficiently small. A simple approximation to this expression (the first few terms of the series) lends itself easily to asymptotic analysis. Furthermore, this approximation was shown to be easily computed numerically.

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