A numerical technique is presented which yields an exact solution to the one-dimensional scattering problem. The algorithm is used to compute phase shift error curves associated with the WKB approximation. A variety of scattering potentials are considered and cover cases for which the WKB solution varies from extremely good to poor. It is shown that some commonly assumed forms for ionospheric electron density profiles yield phase responses which are discontinuous functions of wavenumber. Implications of these results to the inverse scattering problem are discussed.
Phase Shift Errors Associated with the WKB Approximation

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## CONTENTS

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PHASE SHIFT ERRORS ASSOCIATED WITH THE WKB APPROXIMATION

I. INTRODUCTION

In this paper a numerical technique which yields an exact solution to the one-dimensional scattering problem is presented. The method is easy to implement in computer code and it is completely general in that no special assumptions concerning the scattering potential have to be made. Although the procedure is described in terms of a scattering potential, it will be shown that problems dealing with electromagnetic propagation in inhomogeneous, stratified plasmas or dielectrics which are described in terms of an index of refraction can be reformulated in terms of potentials. For the case of wave propagation in plasmas, it turns out the associated potential is proportional to the electron density. The usual method which is applied to general scattering problems is the well known WKB method and the associated connection formulas. A statement for the validity of the WKB approach is that the change of the local wave number over a distance equal to the local wavelength must be small in comparison to the wave number. To apply the connection formulas it is assumed that in the neighborhood of a point where the local wave number is zero the potential can be represented by a linear function with a non-zero slope. There are many interesting problems where these conditions are not satisfied. Given an inhomogeneous plasma or dielectric, as one moves to lower frequency electromagnetic waves, the wavelengths become comparable to the scale of the variation of media properties. If the frequency of the wave is

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such that the index of refraction is approximately zero over a significant path length, then the assumed conditions for the WKB approximation and the connection formulas will not be satisfied.

The orientation of this paper is to investigate the phase error associated with the WKB approximation. It is common in the literature to introduce an additional phase shift of \( \pi/2 \) for reflected waves over and above the phase shift resulting from the geometric optics approximation (see [1]). It has been found that this approach can be fairly accurate even if some of the assumed conditions of the WKB approximation are only approximately satisfied. Conversely, there are also interesting problems for which the WKB approximation introduces a significant error even when the potential is slowly varying relative to the wavelength. One situation for which the WKB method results in large phase errors is a "potential ledge". Ledge type potentials can often be associated with HF propagation in the ionosphere, since the daytime index of refraction for the top of the E-layer is frequently approximately constant for distances up to 50 kilometers. It has also been found that when the scattering potential is in the shape of a well for which there are resonance (metastable) states as discussed by Bohm [2], then the phase error may be quite small except within a very narrow range about the resonance frequency and within this narrow band the phase error fluctuates rapidly. For the case of the ionosphere, a potential well corresponds to a local minimum in the electron density.

The problem to be solved is that of a plane wave incident on a scattering potential. For the corresponding one dimensional problem, the potential is non-zero only in a neighborhood of the origin. The amplitudes and phases of
the reflected and transmitted waves are described by the complex reflection coefficient $R$ and transmission coefficient $T$. The basic situation is a two-sided problem with energy being reflected and transmitted. A one-sided problem can be defined as one in which the scattering potential is such that the transmission coefficient is zero. The technique initially developed is restricted to two-sided problems in that it requires the existence of a non-zero transmission coefficient. However a one-sided problem can be converted into a two-sided problem by "truncating" the scattering potential on the side opposite to the incident wave in such a way that the transmission coefficient is very small, i.e. $|T|^2 \sim 10^{-10}$. In fact, numerical results have shown for this case that $R$ is essentially unchanged as long as the truncation point is chosen such that $|T|^2 \lesssim 10^{-3}$.

Since the scattering of a wave by a known potential is described by a differential equation it seems natural to apply a numerical scheme such as the Runge-Kutta method to obtain an exact solution. A problem arises because the reflection and transmission coefficients are initially unknown and thus the initial conditions necessary for a numerical integration are not available. It is shown that for the original scattering problem there is an associated problem for which the initial conditions on the far side of the scattering potential can be specified. By solving the associated problem and then transforming back to the original problem, one obtains $R$ and $T$.

II. ELECTROMAGNETIC PROPAGATION FORMULATED IN TERMS OF A SCATTERING POTENTIAL

Assume that in a plane stratified medium, the index of refraction is given by $n(x)$ for $-\infty < x < \infty$. For an isotropic plasma, the expression for $n(x)$
is

\[ n^2(x) = 1 - X(x) \]

where \( X(x) \geq 0 \). For a dielectric \( n(x) \) is taken to be

\[ n^2(x) = 1 + \mu^2(x) \]

with \( \mu^2(x) \geq 0 \). Both cases can be described by writing

\[ n^2(x) = 1 + r(x). \]

(1)

The wave equation for propagation in this medium has the form

\[ \nabla^2 W(x,y,z) + k^2 n^2(x) W(x,y,z) = 0. \]

(2)

Here \( k \) is the wave number and is related to the free space wavelength \( \lambda \) by

\[ k = 2 \pi / \lambda . \]

The incident plane wave is given by

\[ W(x,y,z) = u(x) \exp[i k (y \cos \beta + z \cos \gamma)] \]

(3)

where the direction of propagation is defined by the direction cosines \( (\cos \alpha, \cos \beta, \cos \gamma) \). If (3) and (1) are used in (2) we find

\[ \frac{d^2 u}{dx^2} + \left[ E - V(x) \right] u = 0 \]

(4)
where

\[ E = k^2 \cos^2 \alpha \]

\[ V(x) = -k^2 r(x). \]

Except for the constraint on the potential, equation (4) is the one-dimensional Schrodinger equation. For a plasma the scattering potential satisfies

\[ V(x) > 0 \quad \text{all } x, \]

while for a dielectric

\[ V(x) < 0 \quad \text{all } x. \]

III. SOLUTION OF THE SCHRODINGER EQUATION

The equation to be solved is

\[ \frac{d^2 u}{dx^2} + \left[ k^2 - V(x) \right] u = 0. \]  \hspace{1cm} (5)

For simplicity normal incidence of the plane wave is assumed. It is also assumed that \( V(x) \geq 0 \) and \( V(x) = 0 \) outside the interval \((0, L)\). The system to be solved then becomes
\( u(x) = e^{ikx} + Re^{-ikx}, \quad x < 0 \quad (6) \)

\( u(x) = T e^{ikx}, \quad x > L \)

where \( R \) and \( T \) are the unknown reflection and transmission coefficients. A system which is equivalent to (6) is

\[ u(x) = \mu e^{ikx} + \nu e^{-ikx}, \quad x < 0 \]

\[ u(x) = e^{ikx}, \quad x > L \quad (7) \]

Comparison of (6) and (7) shows that \( T = l/\mu \) and \( R = \nu/\mu \). The solution \( u(x) \) can be separated into its real and imaginary parts \( u_r(x) \) and \( u_i(x) \). Both \( u_r(x) \) and \( u_i(x) \) are solutions to Schrödinger equation with

\[ u_r(x) = \cos(kx), \quad x > L \]

\[ u_i(x) = \sin(kx), \quad x > L. \]

The initial conditions for the solutions \( u_r(x) \) and \( u_i(x) \) at \( x = L \) are

\[ u_r(L) = \cos(kL) \]

\[ u_i(L) = -k \sin(kL) \]
and

\[ u_1(L) = \sin(kL) \]
\[ u_1'(L) = k \cos(kL). \]

Both solutions can be projected backwards into the interval \((-2\pi/k, 0)\).

Using the orthogonality of the sine and cosine functions in this interval, the coefficients \(u\), \(v\) and thus \(R\), \(T\) are obtained.

IV. NUMERICAL COMPARISON OF EXACT AND WKB SOLUTIONS

Consider the problem of a plane wave incident from the left on a potential barrier \(V(x)\). As shown in Figure 1, \(V(x)\) is zero for \(x < 0\). The complex wave amplitude \(u(x)\) satisfies equation (5). In terms of the free space wave number \(k\), define

\[ p(x) = \left| k^2 - V(x) \right|^{1/2}, \text{ for } x < a \]
\[ q(x) = \left| V(x) - k^2 \right|^{1/2}, \text{ for } x > a \]

where

\[ V(a) = k^2. \]
Fig. 1 — One-sided scattering potential where incident and reflected waves have free space wavenumber $k$. The classical turning point is $a$. 
The variable \( a \) is called the classical turning point. According to the connection formulas of the WKBJ method, solutions to the left and the right of \( x = a \) are given by

\[
\begin{align*}
    u_1(x) &= \frac{2}{\sqrt{p(x)}} \cos \left[ \int_x^a p(x) \, dx - \frac{\pi}{4} \right] \quad , \quad x < a \\
    u_2(x) &= \frac{1}{\sqrt{q(x)}} \exp \left[ -\int_x^a q(x) \, dx \right] \quad , \quad x > a.
\end{align*}
\]

Consider the region to the left of \( x = a \) and set

\[
A = \int_0^a p(x) \, dx. \quad \text{(9)}
\]

The function \( u_1(x) \) can be expressed as

\[
u_1(x) = u_{\text{in}}(x) + u_{\text{refl}}(x)
\]

where for \( x < 0 \), the incident and reflected waves are

\[
\begin{align*}
    u_{\text{in}}(x) &= \frac{1}{\sqrt{k}} \exp \left[ i \left( \frac{\pi}{4} - A \right) \right] \exp (ikx) \\
    u_{\text{refl}}(x) &= \frac{1}{\sqrt{k}} \exp \left[ i \left( A - \frac{\pi}{4} \right) \right] \exp (-ikx)
\end{align*}
\]

Thus the phase shift of the reflected wave relative to the incident wave at \( x = 0 \) is

\[
\phi_w = 2A - \frac{\pi}{2}.
\]
The final result is that the total phase shift $\phi_w$ predicted by the WKB method is the geometrical optics term $2A$ minus $\pi/2$.

The exact value $\phi_e$ of the phase shift can be obtained from the approach described in section III. The WKB phase shift error

$$E = \phi_w - \phi_e$$

has been computed for several potentials. The first two examples presented are cases where the WKB method is fairly accurate. The first example is a relatively broad quadratic potential barrier of height $E_m = 16$. The barrier width $w$ at half energy value is $10$ free space wavelength, that is

$$w = 10\; \lambda_0$$

where

$$\frac{4\pi^2}{\lambda_0^2} = \frac{1}{2} E_m$$

The potential is shown in Figure 2 and the phase shift error is given Figure 3. It can be seen that the error is only a few degrees over a significant range of wave numbers. Since the quantity $A$ defined by equation (9) approaches 0 as the wavenumber goes to zero, the WKB predicted phase shift is $90^\circ$ for infinitely small wavenumbers. Since the true phase shift approaches $180^\circ$ for small wavenumbers, the limiting value of the phase shift error is $90^\circ$ as the wavenumber goes to 0. This limit has been observed in this and other examples.
Fig. 2 — Broad quadratic potential barrier with half energy width equal to 10 free space wavelengths at corresponding wavenumber
Fig. 3 — Phase shift error for the potential barrier of Fig. 2
The next example considered is the linear potential

\[ V(x) = x. \]

As the wavelength becomes small, it can be seen from Figure 4 that the phase shift error goes to 0. This can be expected since for short wavelengths in a linear potential the assumed conditions for the WKB method and the connection formulas are satisfied.

Several examples where the WKB method has a much larger error will now be described. The first example is a simple modification of the quadratic barrier. The quadratic barrier of Figure 2 is reduced in width so that

\[ W = \lambda_0 \]

where

\[ \frac{4\pi^2}{\lambda_0^2} = \frac{1}{2} E_m \]

Then, as is shown in Figure 5, the phase shift error becomes significantly larger. The increased error can be expected since the potential is a more rapidly varying function of position and also the exponentially decayed form of the wavefunction for \( x > a \) as assumed in equation (8) becomes a poor approximation for narrow barriers.

The potential well shown in Figure 6 has unique phase shift properties. The phase shift error as given in Figure 7 exhibits the typical trend of becoming smaller with decreased wavelength with two exceptions. The exceptions are narrow regions where the phase shift error is an extremely
Fig. 4 — Phase shift error for linear potential $V(x) = x$
Fig. 5 — Phase shift error for a quadratic barrier with half energy width equal to 1 free space wavelength at corresponding wave number.
Fig. 6 — Potential well barrier
Fig. 7 - Phase shift error for the potential of Fig. 6
rapidly varying function of frequency and are associated with the existence
of metastable or resonance states in the terminology of Reference [2]. As
discussed in Reference [2], the condition for the existence of a resonance is

\[ \int_{x_1}^{x_2} \left[ k^2 - V(x) \right]^{1/2} \, dx = (N+1/2) \pi, \text{ for } N = 0, 1, 2, \ldots. \quad (10) \]

Here \( x_1 \) and \( x_2 \) are the classical turning points at the two sides of the
potential well for which

\[ V(x_1) = V(x_2) = k^2. \]

The condition for resonance as specified by equation (10) is again based on
the WKB method. It is worthwhile to compare the accuracy of the WKB
prediction against an exact solution. The exact solution method employed is
based on a finite element scheme applied to the Eigenvalue problem

\[ -\frac{d^2 u}{dx^2} + V(x)u = Eu \]

using Hermite cubic polynomials as basis functions. Here \( V(x) \) is the poten-
tial well shown in Figure 6.

Figure 7 has two "points of discontinuity" where the phase shift error is
essentially a discontinuous function of wave number. Since the WKB predicted
phase shift is for this example a relatively slowly varying function of wave
number, one would expect that these points are wave numbers for which the true
phase shift has a discontinuity. That this is the case can be seen from Figure 8, which shows the true phase shift in a neighborhood of the first point of discontinuity. Using a similar expansion at the higher wave number, these points are determined to four significant figures. The table shown below compares the predicted with the actual location of the points of discontinuity.

<table>
<thead>
<tr>
<th></th>
<th>$k_1$</th>
<th>$k_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Actual</td>
<td>1.608</td>
<td>1.936</td>
</tr>
<tr>
<td>WKB Resonance Condition</td>
<td>1.690</td>
<td>1.942</td>
</tr>
<tr>
<td>Eigenvalue Solution</td>
<td>1.668</td>
<td>1.933</td>
</tr>
</tbody>
</table>

It is interesting to note that for the higher energies and wave numbers one can expect the WKB condition for resonance to become more accurate while the energy eigenvalues determined by a numerical scheme tend to become less accurate. This observation is consistent with results presented above.

The potential obtained from the first hump of the potential well is shown in Figure 9 and the corresponding phase shift error curve is given in Figure 10. It should be noted that except for narrow regions about the two points of discontinuity, the curves in Figures 7 and 10 overlap.
Fig. 8 — Expansion of the phase shift error curve of Fig. 7 about first point of discontinuity
Fig. 9 — Potential barrier obtained from first hump of potential well of Fig. 6
Fig. 10 — Phase shift error for the potential barrier of Fig. 9
In this paper a general technique was presented for computing the complex
reflection and transmission coefficients for a plane wave obliquely incident
on an isotropic and horizontally stratified plasma or dielectric. For a one-

APPROACHES A STEP FUNCTION DISCONTINUITY.

Figure 7 shows the phase response versus the phase shift error. However, as can be seen from
a percentual with a two wavenumber lead, as expected the true phase shift is a
linear percentual with no lead, (2) linear percentual with one wavenumber lead and (3) linear

TURNSING POINT AS THE WAVE NUMBER CROSSES THE LEDGE VALUE OF K = 2. Figure 14

ASSOCIATED WITH A DISCONTINUOUS CHANGE IN THE LOCATION OF THE CLASSICAL
ERROR NEAR THE POINT OF DISCONTINUITY, THE OSCILLATIONS IN THE PHASE ERROR IS
OVER A LONGER PATH LENGTH AND THIS RESULTS IN A MORE WILTY OSCILLATING PHASE
WHERE LEADE, THE CORRESPONDING INDEX OF REFLECTION IS APPROXIMATELY ZERO
LEADE WHOSE WIDTH IS TWO FREE SPACE WAVELENGTHS IS GIVEN IN FIGURE 12. FOR
POPCENTRAL AT THE BEGINNING OF THE LEDGE, THE STEEP OF THE PHASE ERROR FOR A
CONTINUITY AT THE WAVE NUMBER VALUE K = 2 WHICH CORRESPONDS TO THE NEAREST OF THE
DECREASES WITH WAVE NUMBER EXCEPT IN THE NEIGHBORHOOD OF THE POINT OF DISCONT-
ENTS CORRESPONDING TO THE LEDGE HEALTH, THE PHASE ERROR SHOWN IN FIGURE 12
MAXIMUM AT X = 4 AND THE WIDTH OF THE LEDGE IS ONE FREE SPACE WAVELENGTH AT AN
SHOWN IN FIGURE 11 HAS A SMALL CONSERVATIVE SLOPE PAST THE FIRST
THE LAST TWO EXAMPLES PRESENTED ARE LEDGE TYPE POCONENTRALS, THE LEDGE
Fig. 11 — Ledge type potential barrier of width one free space wavelength
Fig. 12 — Phase shift error for a ledge type potential of width one free space wavelength
Fig. 13 — Phase shift error for a ledge type potential of width two free space wavelengths
Fig. 14 — True phase shift for ledge type potentials
and the reflection process is characterized by the phase of the reflection coefficient. The numerical approach is about as easy to implement as the WKB approximation and eliminates the phase errors typically associated with the WKB method. One novel result obtained is that there are commonly occurring index of refraction functions for which the true phase shift of the reflected wave has one or more points of discontinuity. The implications of this type of phase response on communication channels can be explored by doing numerical simulations of pulse propagation taking as the medium transfer function one of unit amplitude and with a discontinuous phase term. As an example, the lower point of discontinuity of Figure 7 is very narrow and in general could not be expected to have any noticeable effect on pulse shape while the upper point of discontinuity is sufficiently broad to significantly change the shape of communication signals. For HF communication, one would want to select a signal bandwidth which avoids the step function discontinuity in the phase response associated with ledges in the electron density profile. As can be seen from Fig. 14, this effect is present even with a relatively narrow ledge corresponding to a width of a few wavelengths.

There are some implications of this study to the plasma inverse problem. Since the phase responses of the potential well and the corresponding single nump potential coincide (see Figures 7 and 10) except at the resonance points, it is apparent that in general no formal solution to the inverse scattering problem can in a practical sense infer the existence of secondary maxima of electron density based on reflected energy. However, in the special case where resonance states occur, the existence of secondary maxima can be investigated by sweeping through a range of frequencies with a narrow band signal and recording the phase shift.
REFERENCES

