An Interactive Code for Solving Differential Equations

Using Phase Integral Methods

R. B. White

Plasma Physics Laboratory, Princeton University

Princeton, N.J. 08540

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ABSTRACT

The solution of ordinary differential equations by the means of Phase Integral Methods is eminently suited for an interactive computational system with real time graphics. We describe a code devised for this purpose and illustrate its use.

I. Introduction

The power and simplicity of Phase Integral Methods¹ for the approximate solution of differential equations make them a common tool in many branches of physics, and a particularly useful one in plasma physics. Unlike the normal situation in Quantum Mechanics where the turning points of the differential equation depend on the eigenvalues in a simple way, in typical plasma physics problems, the turning point locations can be complex functions of the eigenvalue. Because of this, usual methods of solving the differential equation are often not convenient.

It is also the case that the Method of Phase Integrals is particularly suitable for interactive computing. On the one hand Stokes patterns themselves are quite tedious to construct without computational aid, and the integrals determining the eigenvalues often cannot be performed analytically, and on the other hand arriving at a solution involves the recognition of global patterns in Stokes diagrams, and an intuitive understanding of the necessary conditions for the existence of a solution. The pattern recognition and the treatment of the numerous unforeseeable complications which generally accompany an actual physical problem are too complicated to be conveniently written into a code.

The use of Stokes methods for arriving at solutions of arbitrarily complicated differential equations is not without its difficulties. However, almost always in plasma physics

one simply wishes to ascertain whether a normal mode of the canonical two-turning point form exists for various parameter ranges, and if so, to determine approximately its frequency and growth rate. For this canonical problem the use of Stokes methods is straightforward, making a numerical code possible.

In Section II we briefly review the Method of Phase Integrals as it applies to this restricted problem. Section III consists of a general description of the code along with examples of its use.

II. The Method of Phase Integrals

A. Stokes Structure

We take as standard form for the differential equation to be examined

$$\frac{d^2 \psi}{dz^2} + Q(z, \omega) \psi = 0 \quad (1)$$

where ω , the complex frequency, generally plays the role of an unknown eigenvalue, and $z = x + iy$ is a complex variable. The physical problem is initially defined on the real axis and

the equation has been analytically continued into the complex plane. In the case of an algebraically complicated function $Q(z, \omega)$, perhaps dependent on several physical parameters, the job of analyzing the Stokes structure associated with Eq. (1) for all physically interesting parameter values can be quite tedious. Further, the global properties of Stokes regions can change drastically for small changes in the eigenvalue ω . Thus, a means of rapidly exploring this structure in order to ascertain the possibility of the existence of a mode, and in case such a possibility exists to iteratively find the associated frequency ω is extremely useful.

Briefly, as described in Ref. 1, the WKBJ approximate solutions of Eq. (1) take the form

$$\psi_{\pm} = Q^{-1/4} \exp\left(\pm i \int^z Q^{1/2} dz\right) \quad (2)$$

and in certain regions of the complex plane a general solution of Eq. (1) can be approximated by

$$\psi = a_+ \psi_+ + a_- \psi_- \quad (3)$$

The solutions $\psi_{\pm}$ are local, not global solutions of Eq.

(1). First, as is readily verified by substitution in Eq. (1), $\psi_{\pm}$ are approximate solutions only provided that

$$\frac{dQ}{dz} Q^{-3/2} \ll 1 \quad (4)$$

Clearly, this inequality is not valid in the vicinity of a turning point. Aside from this, however, $\psi_{\pm}$ are not approximations of a continuous solution of Eq. (1) in the whole z plane; i.e., the coefficients a_+ , a_- are not fixed over the whole z plane, and the Method of Phase Integrals consists in relating, for a given solution of Eq. (1), the WKBJ approximation in one region of the z plane to that in another.

These regions are separated by the Stokes and anti-Stokes lines associated with $Q(z, \omega)$, and thus the qualitative properties of the solution are determined once these lines are known. We introduce a method of determining these lines which does not involve time consuming integration. Define a local anti-Stokes line to be, for any z_0 , an infinitesimal path emanating from z_0 along which $Q^{1/2} dz$ is real. Along this path $|\psi|$ is essentially constant; i.e., the solution is oscillatory. If $Q(z_0, \omega)$ is finite and well behaved, the local anti-Stokes line is given simply as $dz = \pm Q(z_0)^{-1/2}$; i.e., from z_0 there issue two

oppositely directed lines. Points at which $Q(z_0)$ is zero or infinity must be analyzed with more care. A first order zero, $Q(z) = (z - z_0)$, gives $(z - z_0)^{3/2} = \text{real}$, which has the solution $z - z_0 = \exp(i\pi/3)$; i.e., three lines emanate from the point z_0 instead of two. Similarly, one finds that from a double root there issue four anti-Stokes lines, from a simple pole a single line, etc. It is thus quite easy to read the locations of zeros, poles, etc., of a function from a plot of the z plane upon which are displayed the local anti-Stokes lines. An example is shown in Fig. 1 for a function Q which possesses simple zeros in the first and third quadrants, a double zero in the fourth quadrant, a pole in the second quadrant, and no other zeros or singularities. In referring to Stokes diagrams, we will refer to both zeros and singularities of $Q(z)$ as singular points of the Stokes structure since it is the function $Q^{1/2}$ which is relevant in this diagram.

A display of this nature allows a qualitative survey of the analytic structure of a function, without the numerical complication of an actual search for roots. It is also more convenient than an integral method utilizing closed contours such as that due to Nyquist.

Using the local anti-Stokes lines as guides, we can form global, continuous anti-Stokes lines for those particular lines which emerge from the singular points of the Stokes plot, giving for the example of Fig. 1 the plot of Fig. 2. In

performing these connections, keep in mind that away from the singular points, the lines cannot meet or cross. We similarly define local and global Stokes lines to be lines for which the integral $\int Q^{1/2} dz$ is imaginary. Along the Stokes lines the WKBJ solutions are exponentially increasing or decreasing with fixed phase. Except at singular points the Stokes and anti-Stokes lines are orthogonal. The global anti-Stokes and Stokes lines which are attached to the singular points of the Stokes diagram, along with the Riemann cut lines, describe the global properties of the WKBJ solutions.

As an illustration of a more complicated structure, in Fig. 3 are shown the local anti-Stokes lines associated with the plasma dispersion function² $Z(z)$, defined as the Hilbert transform of the gaussian, $Z(z) = \pi^{-1/2} \int_{-\infty}^{\infty} dt \exp(-t^2) (t-z)^{-1}$ for $\text{Im}z > 0$ and as the analytic continuation of this for $\text{Im}z < 0$.

B. Connection Formulae

The derivation of connection formulae for the WKBJ solutions has a long and involved history, and is not a closed subject. Much is missing in terms of general proofs and analysis of situations with diverse singularities. However, in the domain of mathematical physics, and plasma physics in particular, the vast majority of problems consist in the determination of eigenvalues associated with a potential well of the differential equation. For this case the connection

formula for the approximate harmonic oscillator described by Heading is adequate. Difficulties arise in determining the location of the turning points associated with such a potential well, the evaluation of the integral in the connection formula, which determines the eigenvalue, and the investigation of the topology of the Stokes structure to ascertain whether a global solution can be constructed which has the desired boundary conditions.

The canonical Stokes structure for a solution associated with a pair of real turning points is shown in Fig. 4. For illustration, we have chosen $Q = 100/(z^2 + 1) - \omega$ which has turning points located at $\pm v = \pm \sqrt{100/\omega - 1}$, which are located on the real axis provided ω is real and between zero and 100. In addition to the anti-Stokes lines emanating from the turning points, we have added the Stokes lines (broken lines). There are three separate regions of the real axis where the WKBJ expression can give a good approximation to a solution, and these regions are isolated from one another by the turning points.

In the notation of Heading, ignoring the slow $Q^{-1/4}$ dependence, a WKBJ solution is denoted by

$$(z, v)_s = \exp\left(i \int_v^z Q^{1/2} dz\right) \quad (5)$$

where the subscript s (d) indicates that the solution is subdominant (dominant); i.e., exponentially decreasing (increasing) for increasing $|z - v|$ in a particular region of the z plane, bounded by Stokes and anti-Stokes lines. The point v is taken to be a nearby turning point to which the dominance and subdominance refers. Here increasing $|z - v|$ is made precise by specifying that it signify following the local Stokes lines in the direction that $|z - v|$ increases. The two independent local WKBJ approximate solutions of Eq. (1) in this notation are given by (z, v) and (v, z) . Clearly if (z, v) is subdominant, then (v, z) is dominant. It is readily verified that upon crossing an anti-Stokes line these two solutions reverse character.

The rules given by Heading for obtaining a globally defined WKBJ solution which corresponds to the approximation of a single solution of the differential equation are the following. Begin with a particular solution in one region of the z plane, choosing that combination of subdominant and dominant solutions which gives the desired boundary conditions in this region. The global solution is obtained by continuing this solution through the whole z plane effecting the following changes:

- (1) Upon crossing a Stokes line in a counter clockwise sense, the sense being defined using the singular point from which the line originates as origin, there is a change in the coefficient of the subdominant term. To this coefficient must

be added the term $T^*(\text{dominant term coeff.})$. The Stokes constant T is equal to $+i$ when the singular point is a first order zero of Q .

- (2) Upon crossing a cut in a counter clockwise sense, the cut originating from a first order zero of Q at the point v , we have

$$(v, z) \rightarrow -i(z, v)$$

(6)

$$(z, v) \rightarrow -i(v, z)$$

The property of dominance or subdominance is preserved in this process.

- (3) Upon crossing an anti-Stokes line, subdominant solutions become dominant and vice versa.

These rules describe the results of analytically continuing the WKBJ solutions around the branch points and of integrating Eq. (1) through the turning points, in the neighborhood of which the WKBJ solutions are invalid, but the function Q is dominated by its behavior near the turning point and the integration can be done directly. The connection of the WKBJ solutions can be imagined to be carried out at some distance from the turning point in the complex plane where these solutions are valid. In this manner we can pass from region to region across the cuts and Stokes lines emanating from the turning points. Beginning with any combination of dominant

and subdominant solutions in one region, this process leads to a globally defined single valued approximate solution of Eq. (1). Although it would appear that the first rule gives rise to a discontinuous solution, this is not the case. At the Stokes line, in the presence of a dominant solution, the discontinuity produced is small compared to the error due to the WKBJ approximation itself. As one continues further away from the Stokes line, however, the subdominant term will begin to be important, and the modified coefficient is the correct one.

We illustrate this process for the case of Fig. 4. Assuming that we wish a solution which is exponentially decreasing for $x \rightarrow \infty$, begin in region 1 of Fig. 4 with the subdominant function $(z, v)_s$. Continue directly into region 2 with the change that this function becomes dominant, $\psi = (z, v)_d$. Passing into region 3 we find the continuation

$$\psi = (z, v)_d - i(v, z)_s. \quad (7)$$

To proceed further we attach the solution to the left hand turning point, using the identity

$$(z, c) = (z, a)(a, c) \quad (8)$$

finding also in region 3

$$\psi = (z, -v)_d (-v, v) - i(-v, z)_s (v, -v) . \quad (9)$$

To pass into region 4 we cross a Stokes line in the counter clockwise direction and thus find

$$\psi = -i[(v, -v) + (-v, v)](-v, z)_s + (v, -v)(z, -v)_d \quad (10)$$

and thus in region 5

$$\psi = -i[(v, -v) + (-v, v)](-v, z)_d + (v, -v)(z, -v)_s . \quad (11)$$

Crossing the cut into region 6 we find

$$\psi = [(v, -v) + (-v, v)](z, -v)_d + i(-v, v)(-v, z)_s . \quad (12)$$

In any case, whether we push the cut above the real axis, letting region 5 include it, or leave it as shown in Fig. 4, the connection formula remains the same. Requiring that the solution tend to zero at $x \rightarrow -\infty$, we set the coefficient of the dominant solution equal to zero, or

$$(v, -v) = -(-v, v) \quad (13)$$

which has the solution

$$\int_{-v}^v Q^{1/2} dz = [n + (1/2)]\pi \quad (14)$$

for n integer.

This result is the standard Bohr Sommerfeld condition for the eigenvalue. In this case the solution for $n = 0$ is $\omega = 90.2$. A direct numerical integration of the differential equation gives for $n = 0$ the value $\omega = 90.7$.

For the physical interpretation of the solution and the understanding of the boundary conditions, it is necessary to recall the derivation of the original equation, which is normally through Fourier Laplace transformation of a time dependent equation. The solution for fixed ω is interpretable as a time asymptotic steady state solution. In this particular case the differential equation is self adjoint, there are no sources or sinks of energy, and this is reflected in the Stokes diagram by the fact that the asymptotic x axis exactly coincides with a Stokes line; i.e., the solution is asymptotically exponentially damped, with no propagation in or out. In Section III we present examples in which the differential equation is not self adjoint, and a steady state solution necessitates asymptotic propagation.

III. The Numerical Search for WKBJ Solutions

A. General Description

The code developed is written for interactive use on a console with a screen for plotting. Upon execution of the code, an initial guess for the frequency must be entered and the resulting Stokes structure (local anti-Stokes lines) is displayed. In general, there may be present a number of singular points of various type. If no turning points likely to give a solution of the form desired are observed, a new frequency guess is made and the new Stokes structure is displayed. When a likely pair of turning points are observed, their approximate locations are entered, and the code then locates them to the desired degree of accuracy. Then the integral Eq. (14) is evaluated between these points and the result is displayed. At this point, the desired mode number can be selected, and the code then proceeds to find the correct eigenfrequency iteratively, displaying the resulting Stokes structure, the integration path, the integrand, and the path of the search in the frequency plane. For efficient use of the code, these must all be observed and made use of to arrive quickly at a solution. A more detailed description of the use of this output has been given in a short guide to the actual operation of the code.³

The search routine for the frequency consists of stepping the frequency, by an entered amount, four different directions in the complex plane, and for each step finding the new zeros of $Q(z, \omega)$, calculating the integral, and comparing it to the integral obtained with the original ω . The best resulting ω in terms of satisfying Eq. (14) is then selected for the next iteration. In case none of these stepped values result in a better solution of Eq. (14) than the original value, which will certainly occur when ω is very near the correct eigenvalue, the step distance is decreased and the search is repeated. When improvement of the eigenvalue is impossible, due to errors occurring from the finite number of integration points and the limited accuracy with which the zeros of $Q(z, \omega)$ are found, the frequency search routine will fail and the routine will terminate.

In some cases the turning point locations can be very sensitive functions of ω , and a large step in ω will cause them to be lost. The search for the zeros of $Q(z)$ and the integration paths are displayed during the four-way frequency search, so that if this problem occurs it will be apparent and a smaller value for the frequency step can be selected.

During operation the plot of the integrand indicates how accurately the zeros of $Q(z, \omega)$ are being found; if it is not relatively small at the end points the acceptable error must be reduced. This plot as well as the Stokes plot warns of the presence of zeros or singularities near the integration

path. This is relevant since the integration path must be analytically continuable to a path following the anti-Stokes lines connecting the two turning points. Similarly, the cut structure of $\sqrt{Q(z, \omega)}$ must be taken into account in the continuation of the solution from one region to the next.

The plot of the frequency plane search gives an indication of how rapidly the convergence to the correct eigenvalue is proceeding, and when a value has been bracketed it gives some indication of the accuracy of the determination.

B. Example 1.

Consider the simple example given by

$$Q = -[(\omega^2/2) + 13]/[z^2 + 0.7(1 - i)] - \omega. \quad (15)$$

This is an ad hoc equation which is illustrative of the type of problem encountered in plasma physics. The turning point locations and indeed the validity of the WKBJ approximation depend on the value of the eigenvalue ω , and it is not a priori apparent whether or not solutions exist of the bound state form, nor whether they can be described by Phase Integral Methods. An initial guess of $\omega = 3 + 7i$ gives the Stokes plot shown in Fig. 5. Two turning points exist, and

it appears possible that a solution can be found which exhibits subdominant behavior for $x \rightarrow \pm\infty$. Proceeding with the iteration, we find convergence to an eigenvalue associated with $n = 2$ of $\omega = -1.69 + 8.31i$. The Stokes structure corresponding to this correct eigenvalue is shown in Fig. 6. It is clear that subdominant solutions corresponding to those of regions 1, 6 of Fig. 4 include in their domain of validity the real axis for $x \rightarrow \pm\infty$. As the mode has a positive growth rate the outgoing wave boundary condition corresponds to these asymptotically decaying waves. The form of the solution is essentially the same as that of Fig. 4 with the exception that the Stokes lines do not coincide with the asymptotic real axis and the solution exhibits outwardly propagating waves. The fact that the turning points are complex does not otherwise alter the analysis of the connection formula of Section II. The solution can be regarded as the same, only expressed in a coordinate system which has been rotated and somewhat skewed from that of Fig. 4.

For this particular example the condition for the validity of the WKBJ solution, inequality (4), is fairly well satisfied everywhere on the real axis, as shown in Fig. 7.

C. Example 2.

Consider the equation defined on the real axis by

$$Q = -k^2 + \frac{x^2}{\omega^2 L^2} - \frac{(\omega - 1)}{\omega} [1 + AZ(A)] \quad (16)$$

where

$$A = \frac{\omega L (2R)^{1/2}}{|x|}$$

and L , K , R are real parameters, and Z is the plasma dispersion function. This equation arises in plasma physics in the consideration of the collisionless drift wave. A more complete description of the derivation and solutions of this equation will be reported elsewhere,⁴ for our purposes we may simply regard it as providing an example of interesting complexity. In fact, it has a long history, as initial investigations, relying on approximations of the dispersion function, erroneously predicted a mode with a positive growth rate for large values of K .⁵

The expression $|x|$ arises in a derivation valid on the real axis, and the analytic continuation into the complex plane is provided by $|x| \sim \sqrt{z^2}$. We choose branch cuts along the imaginary axis such that $\sqrt{x^2} \geq 0$ on the physical sheet. For small values of K the term involving the

plasma dispersion function Z is negligible, and two physical sheet turning points are located approximately along the line $x = -y$. As K increases, these turning points begin to migrate toward the imaginary axis. In Fig. 8 is shown the location of the turning points (v and $-v$) for a mode with $L = 50$, $K^2 = 0.07$, and $R = 1/1837$. Note the presence of another pair of turning points (g and $-g$), located on the nonphysical sheet where $\sqrt{x^2} \leq 0$. The eigenvalue determined by the connection formula between v and $-v$ is $\omega = 0.89 - 0.004i$. In this case the mode is decaying, and a solution physically interpretable as steady state must have propagation inward at asymptotically large x . Beginning at large positive x , this requires the choice of a solution which is purely dominant $(z, v)_d$. (The exponential decay toward the origin is associated with the inward propagation.) It is readily verified that the anti-Stokes line emanating from v toward positive x does not cross the real axis. Continuing this solution into region I we thus cross an anti-Stokes line, obtaining $(z, v)_s$, after which the analysis of Section II-B allows the continuation through to a subdominant solution in the upper left quadrant of the physical sheet, which is continued down across the anti-Stokes line to the negative real (x) axis, once again giving a dominant, or inwardly propagating, solution. (If the reader hesitates to pass through the cuts originating at $z = 0$ the problem can be solved entirely in the right half plane by making use of the symmetry of Q .)

As the parameter K increases, an interesting phenomenon occurs. The turning points v , $-v$ as well as the turning points g , $-g$ approach the imaginary axis. For a critical value of $K^2 \approx 0.13$ there is a coalescence, after which the Stokes diagram takes the form of Fig. 9. The role of turning point for the determination of the solution has been passed on from v to g . Once again the analysis presented above carries through, only now the connection formula is determined by performing the integral from g to $-g$. We then discover that the growth $\text{Im}(\omega) = 0$, which can be verified analytically.

It is amusing to note that for K less than the critical value; i.e., for the situation described by Fig. 8, imposing the connection formula between g and $-g$ gives rise to a growing mode $\text{Im}(\omega) > 0$. However, this ghost mode remains on the nonphysical sheet, interpretable as an outwardly propagating solution only on this sheet. The critical value of K is seen to be the coalescence of the turning points of a nonphysical growing mode and a physical damped mode, which annihilate to produce a marginally stable mode for all larger values of K .

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References

1. J. Heading, AN INTRODUCTION TO PHASE INTEGRAL METHODS, John Wiley & Sons.
2. B. D. Fried, C. L. Hedrick, and J. McCune, Phys. Fluids 11, 244 (1968).
3. R. B. White, Princeton Plasma Physics Laboratory preprint PPPL-1408.
4. Liu Chen, P. K. Kaw, C. Oberman, P. Guzdar, and R. B. White. To be published.
5. L. D. Pearlstein and H. L. Berk, Phys. Rev. Lett. 23, 220 (1969). K. T. Tsang, P. J. Catto, J. C. Whitson, and Julius Smith, Phys. Rev. Lett. 40, 327 (1978). David W. Ross and Swadesh M. Mahajan, Phys. Rev. Lett. 40, 324 (1978).

Figure Captions

Fig. 1. Plot of the local anti-Stokes structure for
 $Q = (z - z_1)(z - z_2)(z - z_3)^2/(z - z_4)$ with
 $z_1 = 1 + i$, $z_2 = -1 - i$, $z_3 = 1 - i$, and $z_4 = -1 + i$.

Fig. 2. Same as Fig. 1, with the global anti-Stokes lines added.

Fig. 3. The local anti-Stokes plot for the plasma dispersion function.

Fig. 4. The canonical Stokes structure for an equation with an attractive potential with two real turning points. Shown are the global anti-Stokes (solid) and Stokes (dotted) lines.

Fig. 5. The initial Stokes diagram for the initial frequency guess for the equation of Example 1.

Fig. 6. The Stokes diagram of Example 1 with ω equal to an eigenvalue (that for $n = 2$).

Fig. 7. The WKBJ condition $(dQ/dx)Q^{-3/2}$ along the real axis for the case of Fig. 6. This must be small compared to one for the validity of the WKBJ solutions.

Fig. 8. The Stokes structure for a solution of the equation given in Example 2. Here K^2 is less than the critical value for coalescence of v, g . The turning points $g, -g$ correspond to a mode with positive growth located on the nonphysical sheet. The mode on the physical sheet associated with $v, -v$ is damped.

Fig. 9. The Stokes structure for a solution of the equation given in Example 2. Here K^2 is larger than the critical value and the turning points are located on the imaginary axis. The mode is marginally stable.

Fig. 1. 772575

Fig. 2. 772577

Fig. 3. 772579

Fig. 4. 782036

Fig. 5. 782038

Fig. 6. 782039

Fig. 7. 782040

Fig. 8. 782035

Fig. 9. 782037