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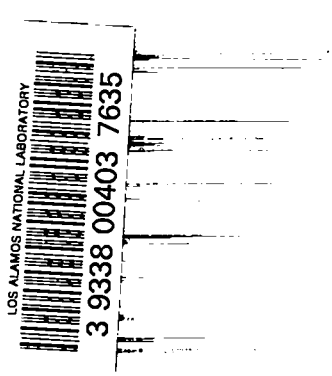
Stability of Detonations for Disturbances of Small Transverse Wavelength



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Stability of Detonations for Disturbances of Small Transverse Wavelength

by

Jerome J. Erpenbeck

ABSTRACT

The stability of one-dimensional, steady detonations to periodic disturbances transverse to the flow is examined in the limit of small wavelength, i.e., $2\pi/\epsilon \to 0$. It is found that any unstable disturbance grows in time t as exp (τt) with $\mathrm{Im}(\tau)/\epsilon$ and $\mathrm{Re}(\tau)$ of order ϵ^0. The asymptotic criterion for stability is found to depend largely upon the steady-state profile of $c_o^2 - u^2$ (where c_o is the frozen sound speed and u is the mass velocity relative to the von Neumann shock) as a function of distance behind the shock. Detonations for which $c_o^2 - u^2$ decreases monotonically are found to be stable (in the $\epsilon \to \infty$ limit), but stability in cases in which this quantity increases either monotonically or up to a maximum (and decreases beyond) is determined through simple integral functions of the steady-flow variables. More complicated profiles are not treated explicitly. In contrast to the labor involved with application of the general theory of detonation stability, the current asymptotic result can be readily applied to any detonation, irrespective of the number of chemical reactions which occur, provided knowledge of the equation of state and reaction kinetics is at hand.

The criterion is applied to an idealized, one-reaction ($A \rightarrow B$) detonation. Unstable regimes are found only if the ratio of specific heats γ_o is less than 2, for which case all detonations are found to be unstable for sufficiently large values of the activation energy. For low heats of reaction, it is found that instability, although not reported in an earlier numerical application of the general theory to long wavelengths, persists for all (positive) heats, unless the activation energy is also small. On the other hand, for more realistic heats of reaction, the present (asymptotic) criterion predicts stability for small activation energies, where long-wavelength,unstable modes were previously found.

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It is my pleasure to thank William W. Wood of this laboratory for many invaluable discussions of the problem of detonation stability and for his helpful criticism of the manuscript for this report. I would also like to express my appreciation to Professor Zevi W. Salsburg of The Rice University for his early interest and discussions concerning this work.

TABLE OF CONTENTS

TABLE OF CONTENTS
(Continued)

LIST OF FIGURES

LIST OF TABLES

GLOSSARY OF SYMBOLS

This glossary contains the principal symbols used in the main text of this report, but does not list those occurring only in the appendices. Symbols which are not included are components of vectors and matrices; these symbols are subscripted versions of the principal symbols, with the overhanging arrow ($\rightarrow$) for a vector or underscore ($\frown$) for a matrix omitted. In the following list, the superscripts and subscripts i and j are understood to take on any positive integer (or zero) value, while ν denotes any signed integer or zero. All other subscripts and superscripts have a specialized meaning.

Symbol	Description	Section Introduced
$a_i(z)$	Polynomial coefficients in the solution of the second-order related equation.	6
$A(z, \hat{\omega})$	Polynomial in $1/\hat{\omega}$ with coefficients $a_i(z)$, entering the solution of the second-order related equation.	6
$\underset{\frown}{A}_x(x)$ $\underset{\frown}{A}_y(x)$	Matrix functions of the steady flow which enters the $\vec{\theta}$ differential equation.	2
$b_1(\tau, \epsilon)$ $b_2(\tau, \epsilon)$	Integrals over the reaction zone involving steady-flow variables and $\vec{\theta}$.	2
$b_i(z)$	Polynomial coefficients in the solution of the second-order related equation.	6
$B(z, \hat{\omega})$	Polynomial in $1/\hat{\omega}$ with coefficients $b_i(z)$, entering the solution of the second-order related equation.	6

GLOSSARY OF SYMBOLS
(Continued)

$\underset{\sim}{B}(x)$	Matrix function of the steady flow which enters the $\vec{\theta}$ differential equation.	2
$c_o(x)$	Frozen sound speed in the steady flow.	3
c_1 } c_2 }	Coefficients of admissible asymptotic solutions in the continuation problem for $\vec{\theta}$.	4
$\vec{c}_i(x)$	Polynomial coefficient in the solution of the $(n + 2)$-order related equation.	6
$\vec{c}(x, \epsilon)$	Polynomial in $1/\epsilon$ with coefficients $\vec{c}_i(x)$ entering as factor in $\vec{\rho}(x, \epsilon)$, the solution of the $(n + 2)$-order related equation.	6
C	Contour of integration for the definition of $\alpha(\epsilon, \zeta, \upsilon)$.	4
$\underset{\sim}{C}(x, \epsilon)$	Matrix of $n + 2$ linearly independent columns $\vec{c}_i(x, \epsilon)$.	6
$d(x)$	Derivative of $c_o^2\eta$ with respect to x in the steady flow.	4
d_1 } d_2 }	Coefficients of admissible asymptotic solutions in the continuation problem for $\vec{\theta}$.	4
$\underset{\sim}{D}(x, \zeta)$	Diagonal matrix, similar to $\underset{\sim}{\Phi}_o(x, \zeta)$.	3
$e(x, \epsilon)$	Correction term in the second-order related equation; the element J_{21} of matrix $\underset{\sim}{J}(x, \epsilon)$.	6
$\hat{e}_i$	Unit vector, having i^{th} element only.	3
$\vec{e}_i(x, \zeta, \upsilon)$	Leading term in the $\vec{\pi}_i$ series in $1/\epsilon$.	3

GLOSSARY OF SYMBOLS
(Continued)

$E^{\ddagger}$	Activation energy for the idealized systems.	7
$\underset{\sim}{E}(x, \zeta, \upsilon)$	A transformed version of $\underset{\sim}{\Phi}_1(x, \upsilon)$.	3
f	Degree of overdrive of the steady idealized detonation.	7
$\vec{f}_i(x, \zeta, \upsilon)$	First correction term in the $\vec{\pi}_i$ series in $1/\epsilon$.	3
$g_i(x)$	Exponential coefficient of $1/\epsilon^i$ in the transformation sequence from $\vec{\theta}$ to $\vec{\psi}$.	6
$\vec{g}_y(x)$, $\vec{g}_t(x)$	Functions of the steady flow which enter the integrands of $b_1(\tau, \epsilon)$ and $b_2(\tau, \epsilon)$.	2
h	Combination of the heat of reaction Q and the heat capacity ratio γ_o for the idealized system.	7
$h_i(x, \zeta)$	Coefficient of ϵ in the exponential of the asymptotic series for $\vec{\pi}_i$.	3
$h_{ij}(x, \zeta)$	$h_i(x, \zeta) - h_j(x, \zeta)$.	3
$\vec{h}_y$, $\vec{h}_t$	Vector functions of the steady detonation, entering into $V(\tau, \epsilon)$.	2
$\mathcal{K}$, $\mathcal{K}_i$	Regions in the complex z-plane.	4
$\underset{\sim}{H}(x)$	Transformed version of $\underset{\sim}{\Phi}_1(x, \upsilon)$.	6
i	$(-1)^{\frac{1}{2}}$.	
$I(x)$	Generic designation for the integrand for $b_1(\tau, \epsilon)$ and $b_2(\tau, \epsilon)$.	5
$I_2(\tilde{z})$	Integrand of the expression for $\beta_2(\zeta_i)$ for the idealized system.	7

GLOSSARY OF SYMBOLS
(Continued)

$\underset{\sim}{I}_i$	Unit matrix of order i.	6
$\underset{\sim}{I}$	$\underset{\sim}{I}_{n+4}$.	2
$j(z)$	Function of longitudinal distance entering the solution of the second-order related equation.	6
$\underset{\sim}{J}(x, \epsilon)$	Correction term in the $(n + 4)$-order related equation.	6
$\hat{k}$	Pre-exponential factor in the Arrhenius rate constant for the idealized system.	7
k_i	Coefficient of $\hat{\omega}^{-1}$ in $k(\hat{\omega})$.	6
$k(\hat{\omega})$	Polynomial in $1/\hat{\omega}$ with coefficients k_i entering the solution of the second-order related equation.	6
k_{00}	The υ independent part of k_0.	6
k_{01}	The coefficient of υ in k_0.	6
$k_i(x, \zeta, \upsilon)$	Coefficient of ϵ^0 in the exponential of the asymptotic series for $\vec{\pi}_i$.	3
$k_i^*(x, \zeta, \upsilon)$	Part of $k_i(x, \zeta, \upsilon)$ which remains finite at the turning point.	5
K	Path of integration from $x = 0$ to ∞.	5
K_0, K_1, K_2	Quantities independent of ϵ and υ_i.	6
$K(\tilde{z})$	Factor of $I_2(\tilde{z})$ for $\beta_2(\zeta_i)$ for the idealized system.	7

GLOSSARY OF SYMBOLS

(Continued)

$\ell(x)$	Function of the steady flow; its value behind the shock enters L_1 and L_2.	5
$\ell_i(x)$	Element 21 of the matrix $-\underset{\sim}{L}_i(x)$, entering the second-order related equation.	6
$L_1(\zeta)$ $L_2(\zeta)$	Contributions to $L(\epsilon, \zeta, \upsilon)$ in the asymptotic limit.	6
$L(\epsilon, \zeta, \upsilon)$	$V(\tau, \epsilon)/\epsilon$ for $\tau = \epsilon\zeta + \upsilon$.	2
$\underset{\sim}{L}_e$	The Onsager matrix of order n.	3
$\underset{\sim}{L}_i(x)$	Coefficient of ϵ^{-i} in the power series for the coefficient matrix for the $\vec{\psi}_{(j)}$, $(j \geq i)$ differential equation.	6
$\underset{\sim}{L}^{(i)}(x, \epsilon)$	Polynomial $\sum_{j=0}^{i-1} \epsilon^{-j}\underset{\sim}{L}_j(x)$.	6
$\underset{\sim}{L}(x, \epsilon)$	$\underset{\sim}{L}^{(m)}(x, \epsilon)$.	6
m	An arbitrary integer, greater than 0, but fixed throughout the discussion in Section 6.	6
M	Generic symbol for a large positive number.	5
$M_{k,p}(\psi)$	Confluent hypergeometric functions.	6
$\underset{\sim}{M}(x, \epsilon)$	Lower (n + 2)-order block of $\underset{\sim}{J}(x, \epsilon)$.	6
n	The integer number of independent chemical reactions.	1
$n(x)$	Function of the steady flow entering $\underset{\sim}{N}_0(x)$.	6
$\underset{\sim}{N}_i(x)$	Lower (n + 2)-order block of $\underset{\sim}{L}_i(x)$.	6

GLOSSARY OF SYMBOLS
(Continued)

$p(x)$	Pressure in the steady detonation.	5
$p_0(z)$ $p_1(z)$	Leading coefficients in the $1/\epsilon$ expansion of the second-order related equation.	6
$P_i(z)$	Paths in the complex z-plane used to establish the admissibility of $\vec{\theta}_i$ solutions.	4
$\underset{\sim}{P}(x, \tau, \epsilon)$	Coefficient matrix of the fundamental $\vec{\theta}$ differential equation.	2
$q(x, \epsilon)$	Power series in $1/\epsilon$ which enters the second-order related equation.	6
$q_i(z)$	Coefficient of $\hat{\omega}^{-i}$ in the power series for $Q(z, \hat{\omega})$.	6
$\tilde{Q}(\gamma_0)$	Transitional value of Q, determined by γ_0.	7
Q	Reduced heat of reaction for the idealized system.	7
$Q^{\ddagger}$	Reduced activation energy for the idealized system.	7
$Q(z, \hat{\omega})$	Transformed version of $q(x, \epsilon)$.	6
$\underset{\sim}{Q}_i(x)$	Transformation matrix, which is part of $\underset{\sim}{S}_i(x, \epsilon)$.	6
$r(x)$	Chemical rate in the steady detonation.	3
$\underset{\sim}{R}_i(x)$	Coefficient of ϵ^{-i} in the power series for $\underset{\sim}{R}(x, \epsilon)$.	6
$\underset{\sim}{R}(x, \epsilon)$	Correction term in the $(n + 4)$-order related equation for $\vec{\varphi}(x, \zeta, \upsilon, \epsilon)$.	6
$s(x, \zeta)$	Square root function of $c_0^2\eta$ and ζ^2.	3
$S(x)$	Specific entropy in the steady flow.	2
S_ν	Sectors of the complex z-plane.	4

GLOSSARY OF SYMBOLS
(Continued)

$\underset{\sim}{S}_i(x, \epsilon)$	Transformation matrix, entering the sequence from $\vec{\theta}$ to $\vec{\psi}$.	6
$\underset{\sim}{S}^{(i)}(x, \epsilon)$	The product $\underset{\sim}{S}_0 \cdot \underset{\sim}{S}_1 \cdots \underset{\sim}{S}_i$.	6
$\underset{\sim}{S}(x, \epsilon)$	$\underset{\sim}{S}^{(m)}(x, \epsilon)$.	6
t	Time.	2
$T(x)$	Temperature in the steady flow.	5
$\underset{\sim}{T}(x, \zeta)$	Transformation matrix which diagonalizes $\underset{\sim}{\Phi}_0(x, \zeta)$.	3
$u(x)$	x component of velocity in the steady detonation, in the frame of reference of the steady shock.	3
$u(z, \hat{\omega})$ $u_\nu(z, \hat{\omega})$	Solution of the second-order related equation.	6
$\vec{u}(x)$	Mass velocity in the steady flow with components $u(x)$ and 0.	2
$\underset{\sim}{U}_i^{(j)}(x)$	Coefficient of ϵ^{-i} in the power series for $\underset{\sim}{U}^{(j)}(x, \epsilon)$.	6
$\underset{\sim}{U}^{(j)}(x, \epsilon)$	Portion of coefficient matrix of the $\vec{\psi}_{(j)}$ differential equation not in the block-diagonal form of $\underset{\sim}{L}^{(j)}(x, \epsilon)$.	6
$\underset{\sim}{U}_i(x)$	$\underset{\sim}{U}_i^{(m)}(x)$.	6
$\underset{\sim}{U}(x, \epsilon)$	$\underset{\sim}{U}^{(m)}(x, \epsilon)$.	6
$v(x)$	Specific volume in the steady flow.	6
$v_\nu(z, \hat{\omega})$	Contribution to $u_\nu(z, \hat{\omega})$ in the second-order related equation.	6

GLOSSARY OF SYMBOLS
(Continued)

$V(\tau, \epsilon)$	Fundamental function whose roots in the τ-plane determine stability.	1
$W(\tau, \epsilon)$	Contribution to the shock distortion from the initial perturbations.	2
$W_\nu[\psi, k(\hat{\omega})]$	A solution of the confluent hypergeometric differential equation.	6
$W_{k,p}(\psi)$	Whittaker functions.	6
$W_\nu(\psi)$	Variant of $W_{k,\frac{1}{4}}(\psi)$.	6
x	Longitudinal coordinate in the frame of reference of the steady shock.	2
x^*	Value of x at a turning point.	3
x_1^*	The greater of a pair of turning points.	4
x_o	Particular value of x.	3
$X_{12}(x)$	Function of the steady flow entering $\alpha(\epsilon, \upsilon)$.	6
y	Spatial coordinate transverse to the steady flow.	2
$y(x, \epsilon)$ $y_i(x, \epsilon)$	Component 1 of $\vec{y}(x, \epsilon)$ or $\vec{y}_i(x, \epsilon)$; solutions of the second-order related equation.	6
$\vec{y}(x, \epsilon)$ $\vec{y}_i(x, \epsilon)$	Solutions of the $(n + 4)$-order related equation.	6
z	Spatial variable derived from x. Except in Section 6, it denotes the analytic continuation of x to the complex plane. In Section 6, it represents $x - x^*$.	4

GLOSSARY OF SYMBOLS
(Continued)

$\hat{z}$	Variable of integration, replacing x, used in several contexts.	5
$\tilde{z}(\zeta)$	Variable of integration for $\beta_2(\zeta_i)$ for the idealized system.	7
$\alpha(\epsilon, \zeta, \upsilon)$	Coefficient of the μ_2-type contribution to $\vec{\theta}$ for turning points associated with profiles M and I.	5
$\alpha(\epsilon, \upsilon)$	Function having the properties of $\alpha(\epsilon, \zeta, \upsilon)$, but for the turning point at the maximum of profile M.	6
$\beta(\epsilon, \zeta, \upsilon)$	$\ell n\, \alpha(\epsilon, \zeta, \upsilon)$.	5
$\beta_1(\zeta_i)$	Coefficient of $-i\epsilon$ in $\beta(\epsilon, \zeta, \upsilon)$.	5
$\beta_2(\zeta_i)$	Contribution to $\beta(\epsilon, \zeta, \upsilon)$ independent of ϵ and υ.	5
$\beta_3(\zeta_i)$	Coefficient of $-\upsilon$ in $\beta(\epsilon, \zeta, \upsilon)$.	5
γ_o	Ratio of specific heats for the idealized system.	7
$\Gamma(a)$	Gamma function.	6
δ	Either i or 1, depending on whether the steady detonation has a maximum or minimum at the extremum of $c_o^2\eta$.	6
$\Delta(x, \zeta, \upsilon)$ $\Delta_1(\hat{z})$ $\Delta_2(\hat{z})$ $\Delta_4(\hat{z})$	Factors in the asymptotic expressions for the integrands of $b_1(\tau, \epsilon)$ and $b_2(\tau, \epsilon)$.	5
ϵ	Wave number of the disturbance (times 2π) in the transverse spatial coordinate y.	1

GLOSSARY OF SYMBOLS
(Continued)

ζ	Leading term in the assumed dependence of τ on ϵ; $\tau = \epsilon\zeta + \upsilon$.	2
ζ_i	$\mathrm{Im}(\zeta)$.	2
$\eta(x)$	Sonic parameter in the steady flow.	3
$\vec{\theta}(x, \tau, \epsilon)$ $\vec{\theta}(x, \zeta, \upsilon, \epsilon)$	Bounded solution, as $x \to \infty$, of the fundamental differential equation.	2
$\vec{\theta}_i(x, \zeta, \upsilon, \epsilon)$	Solution of the fundamental differential equation, irrespective of the boundedness condition.	3
$\vec{\theta}_i^{(\nu)}(x, \zeta, \upsilon, \epsilon)$	Series expression for $\vec{\theta}_i$, analytically continued around a turning point to sector S_ν.	4
$\kappa(x)$	Mach number in the steady flow.	3
κ_{-t}	Shock Mach number for idealized detonations marking the transition from profile M to profile I behavior.	7
$\lambda(x)$	Progress variable in the steady flow for the idealized system.	7
$\vec{\lambda}(x)$	Progress variable in the steady flow.	2
$\underset{mi}{\Lambda}_i(x, \epsilon)$	Coefficient matrix for the $\vec{\psi}_{(i)}$ differential equation.	6
$\mu^{(i)}(\zeta, \upsilon)$	Coefficient of ϵ^{-i+1} in the power series expansion of the eigenvalues of $-\underset{m}{P}'(\infty, \zeta\epsilon + \upsilon, \epsilon)$ in $1/\epsilon$.	4

GLOSSARY OF SYMBOLS

(Continued)

$\mu_i(x, \zeta)$	Eigenvalue of $\underset{\sim}{\Phi}_0(x, \zeta)$.	3
$\mu_{ij}(x, \zeta)$	$\mu_i(x, \zeta) - \mu_j(x, \zeta)$.	4
ν_v	Compression ratio v_+/v_- for the steady shock.	5
$\vec{\nu}^{(i)}(\zeta, \upsilon)$	Coefficient of ϵ^{-i} in the power series expansion of the eigenvector of $-\underset{\sim}{P}'(\infty, \zeta\epsilon + \upsilon, \epsilon)$.	4
$\zeta(\lambda)$	Monotone function of the progress variable for the idealized system.	7
ζ_e	Value of $\zeta(\lambda)$ at chemical equilibrium; $\zeta(0)$.	7
ζ^*	Value of $\zeta(\lambda)$ at the turning point.	7
$\zeta(\tau, \epsilon)$	Fourier-Laplace transform of the shock distortion.	2
$\vec{\pi}(x, \zeta, \upsilon, \epsilon)$	$\underset{\sim}{T}(x, \zeta)^{-1} \cdot \vec{\theta}(x, \zeta, \upsilon, \epsilon)$.	3
$\vec{\pi}_i(x, \zeta, \upsilon, \epsilon)$	$\underset{\sim}{T}(x, \zeta)^{-1} \cdot \vec{\theta}_i(x, \zeta, \upsilon, \epsilon)$.	3
$\Pi(z)$	Factor in the solutions of the second-order related equation, $u_\nu(z, \epsilon)$.	6
$\vec{\rho}(x, \epsilon)$	Solution of the $(n + 2)$-order related equation.	6
$\sigma(\nu)$	$(-1)^\nu$.	6
$\vec{\sigma}(x)$	Thermodynamic function in the steady flow.	3
Σ_ν	Sector in the complex ψ-plane.	6
$\Sigma(z, \hat{\omega})$	Combination of coefficients in the second-order related equation.	6

GLOSSARY OF SYMBOLS
(Continued)

τ	Laplace time transform parameter.	1
υ	Part of τ assumed independent of ϵ.	2
υ_i	$\mathrm{Im}(\upsilon)$.	6
$\Upsilon(z, \hat{\omega})$	Factor in the solutions of the second-order related equation $u_\nu(z, \hat{\omega})$.	6
φ	$\arg(z - x^*)$.	4
$\bar{\varphi}$	$\arg(x^* - z)$.	4
$\phi(z)$	$p_0(z)^{\frac{1}{2}}$.	6
$\varphi_i(\hat{z})$	Integrals of $\mu_1(x, \zeta)$ and $\mu_2(x, \zeta)$, entering the asymptotic expressions for $b_1(\tau, \epsilon)$ and $b_2(\tau, \epsilon)$.	5
$\vec{\varphi}(x, \zeta, \upsilon, \epsilon)$	Solution of the $(n+4)$-order related equation.	6
$\underset{\sim}{\Phi}_0(x, \zeta)$	Leading term in ϵ of $-\underset{\sim}{P}'(x, \zeta\epsilon + \upsilon, \epsilon)$.	2
$\underset{\sim}{\Phi}_1(x, \zeta)$	Part of $-\underset{\sim}{P}'(x, \zeta\epsilon + \upsilon, \epsilon)$ independent of ϵ.	2
$\psi(t, \epsilon)$	Fourier transform of $\Psi(y, t)$.	2
$\Psi(y, t)$	Distortion of the shock.	2
$\Psi(z, \hat{\omega})$	Stretched coordinate in the second-order related equation.	6
$\vec{\psi}_{(i)}(x, \epsilon)$	Transform of $\vec{\theta}(x, \zeta, \upsilon, \epsilon)$ by $\underset{\sim}{S}^{(i)}(x, \epsilon)$.	6
$\vec{\psi}(x, \epsilon)$	$\vec{\psi}_{(m)}(x, \epsilon)$.	6
$\vec{\psi}_i(x, \epsilon)$	Independent solutions of the $\vec{\psi}$ differential equation.	6

GLOSSARY OF SYMBOLS
(Continued)

ω	Parameter for the idealized system determined by detonation velocity and γ_o.	7
$\hat{\omega}$	Large parameter, $\delta\epsilon$.	6
Ω	Parameter for the idealized system determined by detonation velocity and γ_o.	7
$\aleph$ $\aleph_i$	Interval of the real x axis on which $\underset{\sim}{T}(x, \zeta)$ is differentiable.	3

Subscripts

+	Evaluation in the steady flow, behind the shock.	5
-	Evaluation in the steady flow, in front of the shock.	5
max	Evaluation at the point in the steady flow where $c_o^2\eta$ is maximum.	4
CJ	Evaluation for the Chapman-Jouguet detonation velocity.	7

1. INTRODUCTION

The phenomenon of detonation has been the subject of continuing theoretical analysis ever since the pioneering work in the nineteenth century. As a result of a certain amount of agreement between theory and experiment, this effort resulted in the general acceptance of the so-called von Neumann-Zeldovich-Doering theory. The fundamental notion in this theory is that the phenomenon consists of a shock propagating into the quiescent material, with a resultant initiation of exothermic chemical reaction behind this front. A quantitative description of the structure of the detonation wave is presumably complicated in its early stages, but the theory directs its attention to the situation after all transients arising from the initiation of the detonation have vanished. It is supposed, then, that the detonation ultimately becomes a steady, one-dimensional flow when viewed in the frame of reference of the shock. The investigation of the consequences of these assumptions, with particular attention to the Chapman-Jouguet hypothesis for the determination of the velocity of the shock front, has been a principal concern of theoretical endeavors in this field.

Beginning approximately in 1959 the experimental evidence was increasingly seen to be not entirely compatible with the above picture. In

particular, numerous instances of three-dimensional structure of an apparently non-transient nature have been reported.[1, 2]

From a theoretical point of view, the possibility, that the supposed one-dimensional, steady detonations do not actually occur, is subject to analytic investigation. The author[3] has attempted to determine the so-called hydrodynamic stability of steady detonations; that is, whether or not small disturbances imposed upon the steady flow at some instant will die out with time. Should any infinitesimal disturbance grow, the detonation is said to be hydrodynamically unstable.

The key to the hydrodynamic-stability theory is that the equations of reactive hydrodynamics are linearized in the deviations of the perturbed flow from the steady flow. By virtue of this, the dependence of the perturbations on the coordinates transverse to the steady flow is removed by Fourier decomposition and one is left with the stability problem for a given transverse wave number $\epsilon/2\pi$.

Now the general theory of detonation stability[3] can be carried to the definition of a criterion based upon the roots in the complex τ-plane of a certain function V of τ, ϵ, and the steady flow. The determination of $V(\tau, \epsilon)$ for a given steady flow is by no means simple, requiring the solution of a system of ordinary differential equations of order $n + 4$ (for detonations involving n independent chemical reactions) whose coefficients depend upon the steady-detonation structure in the reaction zone as well as τ and ϵ. Ordinarily, then, the stability problem is expected to require numerical solution with results, therefore,

limited to a finite range of wave numbers. A recent calculation[4] for an ideal-gas, unimolecular-reaction system was able to establish instability of certain detonations over finite ranges of ϵ. However, any assertion of the stability of a given detonation was necessarily qualified to include only those values of ϵ which were numerically accessible to the calculation. Thus, we are led to investigate the stability criterion in the limit of small wavelength, i.e., large ϵ.

Since the present theory neglects the transport effects of diffusion, viscosity, and heat conduction, the unit of length in the problem is determined by the gradients in the steady flow. Hence, the analysis of the $\epsilon \to \infty$ limit is expected to apply to wavelengths which are short relative to the reaction-zone length.† On the other hand, transport effects are expected to become important, at least for finite disturbance magnitudes, for wavelengths comparable to a mean free path. Although the validity of our theory cannot be ascertained without recourse to the transport equations, it is not unreasonable to suppose the restriction of our present considerations to wavelengths which are long relative to a mean free path and short relative to the reaction-zone length to be physically meaningful.

The mathematical considerations which are attendant upon the investigation of the $\epsilon \to \infty$ limit are those of the so-called parameter

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† The reaction zone is formally of infinite extent. The phrase "reaction-zone length" refers, of course, to any convenient measure of the region over which state variables change substantially, e.g., the distance to half-completion of some reaction.

problem for linear differential equations. This branch of analysis is essentially complete for systems of differential equations of any order, provided there are no so-called turning points, but is limited to certain second-order equations and specific high-order equations when a turning point is involved. For large systems of equations there does not seem to be any appreciable analysis in the literature for the turning-point problem.

Turning points of rather simple types play a central role in the analysis of the small-wavelength limit, so that we require that the small, but troublesome, gap associated with the $(n + 4)$-order system of equations first be bridged. A large portion of this report is involved with precisely this problem.

After establishing asymptotic expressions for the desired function $V(\tau, \epsilon)$, the stability of the idealized system previously investigated[4] is examined in the small-wavelength limit.

2. RESUMÉ OF THE GENERAL THEORY

The time evolution of an initial perturbation from a steady detonation, moving along the x axis, is reflected by the secular behavior of the distortion $\Psi(y, t)$ of the leading shock. If x is the coordinate in the direction of the steady-state flow and the origin $(x = 0)$ is located in the (distorted) shock, while y is the coordinate transverse to the steady wave,† then $- \Psi(y, t)$ is the x coordinate of the

†For brevity, we use only one transverse coordinate. The stability criterion is identical to that for three dimensions.[3]

unperturbed shock at time t. The general theory of detonation stability[3] has shown that for infinitesimal disturbances the Fourier transform of $\tilde{\psi}$ on the transverse coordinate has its Laplace time transform

$$\psi(t, \epsilon) = \int_{-\infty}^{+\infty} e^{-i\epsilon y} \tilde{\psi}(y, t)\, dy \tag{2.1}$$

given by

$$\xi(\tau, \epsilon) = \int_0^{\infty} e^{-\tau t} \psi(t, \epsilon)\, dt$$

$$= W(\tau, \epsilon)/V(\tau, \epsilon). \tag{2.2}$$

The function $W(\tau, \epsilon)$ is determined by the ϵ-Fourier component of the initial perturbations in the state variables [say, specific volume v, mass velocity $\vec{u}$ (a 2-vector), specific entropy S, and chemical composition $\vec{\lambda}$ (an n-vector)] throughout all of space, and has been shown to contain no singularities in the right half τ-plane.

The function V depends upon the steady flow but not on the initial perturbations. It is given explicity by

$$V(\tau, \epsilon) = \tau b_1(\tau, \epsilon) + i\epsilon b_2(\tau, \epsilon) - \vec{\theta}(0, \tau, \epsilon) \cdot (\tau \vec{h}_t + i\epsilon \vec{h}_y),$$

$$b_1(\tau, \epsilon) = \int_0^{\infty} \vec{\theta}(x, \tau, \epsilon) \cdot \underset{\sim}{A}_x^{-1}(x) \cdot \vec{g}_t(x)dx \tag{2.3}$$

$$b_2(\tau, \epsilon) = \int_0^{\infty} \vec{\theta}(x, \tau, \epsilon) \cdot \underset{\sim}{A}_x^{-1}(x) \cdot \vec{g}_y(x)dx.$$

The vector function $\vec{\theta}(x, \tau, \epsilon)$ is the solution of the differential equation

$$\frac{d\vec{\theta}}{dx} = - \underset{\sim}{P}'(x, \tau, \epsilon) \cdot \vec{\theta}$$

$$\underset{\sim}{P}(x, \tau, \epsilon) = - \underset{\sim}{A}_x^{-1}[\tau \underset{\sim}{I} + i\epsilon \underset{\sim}{A}_y(x) + \underset{\sim}{B}(x)] \tag{2.4}$$

which is bounded in the reaction zone for $\mathrm{Re}(\tau) > 0$; i.e.,

$$\vec{\theta}(x, \tau, \epsilon) = O(1) \text{ as } x \to \infty \text{ for } \mathrm{Re}(\tau) > 0. \tag{2.5}$$

The prime denotes the transpose matrix. The vectors $\vec{\theta}$, $\vec{g}_t$, $\vec{g}_y$, $\vec{h}_t$, and $\vec{h}_y$ are $(n + 4)$-vectors, one component for each state variable, while $\underset{\sim}{A}_x(x)$, $\underset{\sim}{A}_y(x)$, $\underset{\sim}{B}(x)$, and $\underset{\sim}{I}$ are $(n + 4)$-order square matrices; $\underset{\sim}{I}$ is the unit matrix and the remainder of these quantities (given in Ref. 3) are completely determined by the steady detonation, with $\vec{h}_t$ and $\vec{h}_y$ being determined solely by the von Neumann shock itself, i.e., by the equation of state of the unreacted explosive and the steady detonation velocity.

The occurrence of instability, in the sense of exponentially growing contributions to $\psi(t, \epsilon)$, is seen to be occasioned by roots of $V(\tau, \epsilon)$ lying in the right half τ-plane. The problem of detonation stability resolves into determining whether or not V has such roots. The only general result in this regard is the fact that for $|\tau|$ large (at fixed values of the detonation velocity and ϵ) with $\mathrm{Re}(\tau) \geq 0$, V is of order $|\tau|^2$ and has no roots at infinity.

Now in obtaining $V(\tau, \epsilon)$ asymptotically in ϵ, it is of importance that the magnitude of τ be permitted to depend on ϵ, the dependence being such as to reproduce the asymptotic dependence of the roots of V on ϵ. For this purpose, we let

$$\tau = \epsilon\zeta + \upsilon \tag{2.6}$$

whence Eq. (2.3) and (2.4) become

$$V(\tau, \epsilon) = \epsilon L(\epsilon, \zeta, \upsilon)$$

$$L(\epsilon, \zeta, \upsilon) = \zeta b_1 + ib_2 - \vec{\theta}(0, \zeta, \upsilon, \epsilon) \cdot [\zeta\vec{h}_t + i\vec{h}_y] \tag{2.7a}$$

$$+ \epsilon^{-1}\upsilon\,[b_1 - \vec{\theta}(0, \zeta, \upsilon, \epsilon) \cdot \vec{h}_t]$$

$$\frac{d\vec{\theta}}{dx} = [\epsilon\underset{\sim}{\Phi}_0(x, \zeta) + \underset{\sim}{\Phi}_1(x, \upsilon)] \cdot \vec{\theta}$$

$$\underset{\sim}{\Phi}_0 = [\underset{\sim}{A}_x^{-1} \cdot (\zeta\underset{\sim}{I} + i\underset{\sim}{A}_y)]' \tag{2.7b}$$

$$\underset{\sim}{\Phi}_1 = [\underset{\sim}{A}_x^{-1} \cdot (\upsilon\underset{\sim}{I} + \underset{\sim}{B})]'$$

$$\vec{\theta} = O(1) \quad \text{as } x \to \infty, \text{ for } \mathrm{Re}(\tau) > 0\ . \tag{2.7c}$$

The significance of the substitution, Eq. (2.6), is that the leading term of $\vec{\theta}$ (as $\epsilon \to \infty$) depends, as we shall see, upon both $\underset{\sim}{\Phi}_0$ and $\underset{\sim}{\Phi}_1$, and any unstable roots of the leading term of $V(\tau, \epsilon)$ occur on the axis $\mathrm{Re}(\zeta) = 0$. Thus, the sign of the real part of υ will determine whether such roots are stable.

3. FORMAL SOLUTIONS

In this section, we obtain, following the theory of the parameter problem,[5] the leading terms in the ϵ-asymptotic solutions of Eq. (2.7b). The validity of these expressions in the asymptotic representation of $\vec{\theta}$ will be the concern of Section 4.

Series solutions of Eq. (2.7b) are obtained from diagonalization of the leading matrix $\underset{\sim}{\Phi}_0$. If there exists a similarity transform $\underset{\sim}{T}(x, \zeta)$, differentiable on an x interval $\aleph$, such that

$$\underset{\sim}{T}^{-1} \cdot \underset{\sim}{\Phi}_0 \cdot \underset{\sim}{T} = \underset{\sim}{D}(x, \zeta) = \mathrm{Diag}(\mu_1, \mu_2, \ldots, \mu_{n+4}) \tag{3.1}$$

(the second equality denoting that $\underset{\sim}{D}$ is diagonal and defining its elements), then the transformation of $\vec{\theta}$ by $\underset{\sim}{T}^{-1}$ yields the system of equations,

$$\vec{\pi} = \underset{\sim}{T}^{-1} \cdot \vec{\theta}$$

$$\frac{d\vec{\pi}}{dx} = (\epsilon \underset{\sim}{D} + \underset{\sim}{E}) \cdot \vec{\pi} \tag{3.2}$$

$$\underset{\sim}{E}(x, \zeta, \upsilon) = \underset{\sim}{T}(x, \zeta)^{-1} \cdot [\underset{\sim}{\Phi}_1(x, \upsilon) \cdot \underset{\sim}{T}(x, \zeta) - d\underset{\sim}{T}(x, \zeta)/dx].$$

Following the scheme given by Friedrichs,[5] we substitute[†]

$$\vec{\pi}_i = [\vec{e}_i(x, \zeta, \upsilon) + \epsilon^{-1}\vec{f}_i(x, \zeta, \upsilon) + \ldots] \exp [\epsilon h_i(x, \zeta) + k_i(x, \zeta, \upsilon)] \tag{3.3}$$

in which subscript i distinguishes among the solutions which will arise. The unknowns h_i, $\vec{e}_i$, k_i, $\vec{f}_i$ ... are found by equating powers of ϵ in Eq. (3.2); one obtains

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[†]The factor exp (k_i) is not separated from $\vec{e}_i$ and $\vec{f}_i$ by Friedrichs, but this is not a consequential difference.

$$h_i(x, \zeta) = \int_0^x \mu_i(x', \zeta)\, dx' \tag{3.4}$$

but the determination of the remaining quantities depends largely upon whether or not the eigenvalues, μ_i, are distinct. The solution $\vec{\pi}_i$ is said to be of the μ_i type.

The eigenvalue-eigenvector problem for $\underset{\sim}{\Phi}_0$ can be solved explicitly and, in fact, is similar to that which occurs in the problem of shock stability.[6] In Appendix A, we compute $\underset{\sim}{\Phi}_0$ and find its eigenvalues to be

$$\begin{aligned} \mu_1 &= -\kappa(\kappa\zeta + s)/\eta u \\ \mu_2 &= -\kappa(\kappa\zeta - s)/\eta u \\ \mu_3 &= \mu_4 = \cdots = \mu_{n+4} = \zeta/u \\ s &= [\zeta^2 + c_o^2\eta]^{\frac{1}{2}} . \end{aligned} \tag{3.5}$$

The notation of Eq. (3.5) is as follows: $\eta(x)$ is the sonic parameter

$$\eta = 1 - u^2/c_o^2$$

in which $c_o(x)$ is the frozen sound speed and $u(x)$ is the mass velocity in the steady frame of reference; $\kappa(x)$ is the local Mach number u/c_o. The square root $s(x, \zeta)$ is to be understood as a function of ζ with parametric dependence of x, whence it suffices to specify that s is the positive branch of the function with a branch cut along the imaginary ζ axis between $\pm ic_o\eta^{\frac{1}{2}}$. The matrix of right eigenvectors $\underset{\sim}{T}$ and its inverse are also given in Appendix A, along with certain elements of $\underset{\sim}{E}$ which will be required.

Now in the subsonic reaction zone, we see from Eq. (3.5) that only μ_1 has, for $\mathrm{Re}(\zeta) > 0$, negative real part. It is not surprising that $\vec{\pi}_1$ will be of primary importance in finding $\vec{\theta}$ since the latter must satisfy the boundary condition Eq. (2.7c). The determination of the unknowns in $\vec{\pi}_1$ is straightforward;

$$\vec{e}_1(x, \zeta, \upsilon) = \hat{e}_1$$

$$dk_1(x, \zeta, \upsilon)/dx = E_{11}(x, \zeta, \upsilon) \tag{3.6}$$

$$k_1(x, \zeta, \upsilon) = \int_{x_o}^{x} E_{11}(x', \zeta, \upsilon)dx'$$

where $\hat{e}_j$ denotes the unit vector having only its j^{th} component non-zero. The lower limit of integration x_o need only be selected on the $\aleph$ interval in order to ensure existence of the integral. The next-order term is found to be

$$\vec{f}_1(x, \zeta, \upsilon) = -\begin{bmatrix} \sum_{j=2} \int_{x_o}^{x} dx' E_{1j}E_{j1}/(\mu_j - \mu_1) \\ E_{21}/(\mu_2 - \mu_1) \\ E_{31}/(\mu_3 - \mu_1) \end{bmatrix} . \tag{3.7}$$

where x_o is not necessarily the same as in Eq. (3.6) but does lie on $\aleph$. Higher terms are readily written down for this series.

Now it will be convenient to denote the solutions of Eq. (2.7b), irrespective of the boundary condition Eq. (2.7c), by subscripted symbols $\vec{\theta}_i$ as determined by the inverse transform from $\vec{\pi}_i$. As we noted, then $\vec{\theta}_1$ is bounded in x for $\mathrm{Re}(\zeta) > 0$. For $\mathrm{Re}(\zeta) = 0$, μ_1 has negative real part for x large only if $|\mathrm{Im}(\zeta)| < (c_o \eta^{\frac{1}{2}})_{x=\infty}$. For pure imaginary ζ of greater magnitude, it is seen that $\vec{\theta}_1$ is bounded if E_{11} has a non-vanishing, negative, real part. From Appendix A, Eq. (A.16), we find, using linearization of the reaction rate $\vec{r}$ near equilibrium,[7]

$$E_{11}(\infty, \zeta, \upsilon) = \left\{ -\frac{\kappa(\zeta + \kappa s)}{2us\eta} \left[2\upsilon + c_o^2 \vec{\sigma} \cdot \underset{\sim}{L}_e \cdot \vec{\sigma} \right] \right\}_{x=\infty} \tag{3.8}$$

where $\underset{\sim}{L}_e$ is the symmetric, positive-definite, Onsager matrix (order n) and $\vec{\sigma}$ is a thermodynamic function, related to the heat of reaction.[7] It follows that, for $\mathrm{Re}(\zeta) = 0$, $|\zeta| > (c_o \eta^{\frac{1}{2}})_{x=\infty}$, and $\mathrm{Re}(\upsilon) \geq 0$, we have

$$\mathrm{Re}[E_{11}(\infty, \zeta, \upsilon)] < 0. \tag{3.9}$$

Therefore, $\vec{\theta}_1$ is bounded as $x \to \infty$ for all $\mathrm{Re}(\tau) \geq 0$ [except, of course, for $\zeta = \pm i(c_o \eta^{\frac{1}{2}})_{x=\infty}$, for which the interval of definition $\aleph$ must be bounded away from $x = \infty$].

Although $\vec{\theta}_1$ has the desired boundedness property, it will be seen that $\vec{\theta}_2$ is also required explicitly. The evaluation of the latter is evident from our expressions for $\vec{\theta}_1$. Thus

$$\vec{\pi}_2 = [\hat{e}_2 + \epsilon^{-1}\vec{f}_2 + \ldots] \exp [\epsilon h_2(x, \zeta) + k_2(x, \zeta, \upsilon)]$$

$$h_2 = \int_0^x \mu_2(x', \zeta)dx' \tag{3.10}$$

$$k_2 = \int_{x_o}^x E_{22}(x', \zeta, \upsilon)dx'.$$

The other solutions $\vec{\theta}_3$, $\vec{\theta}_4$, ..., $\vec{\theta}_{n+4}$, all of the μ_3 type, need not concern us other than the fact that their series exist; the prescription given by Friedrichs[5] applies to this degenerate case as well, although explicit determination of $\vec{\pi}_3$, ... in terms of elementary functions is not generally possible.

The region of definition of the $\vec{\theta}_i$ depends upon the existence and differentiability of the transform $\underset{\sim}{T}(x, \zeta)$. As is seen from Appendix A, the intervals $\aleph$ can be terminated only at a point x^* at which $s(x^*, \zeta)$ vanishes or where $u(x^*) = \zeta$. It is convenient then to classify the values of ζ according to the properties of the matrix $\underset{\sim}{T}$:

$$\begin{aligned}
&\text{Class III:} \quad \mathrm{Re}(\zeta) = 0 \text{ and } \min_x (c_o\eta^{\frac{1}{2}}) \le |\zeta| \le \max_x (c_o\eta^{\frac{1}{2}}),\\
&\text{Class II:} \quad \mathrm{Im}(\zeta) = 0 \text{ and } \min_x (u) \le \zeta \le \max_x (u),\\
&\text{Class I:} \quad \text{All other } \zeta, \text{ with } \mathrm{Re}(\zeta) \ge 0.
\end{aligned} \tag{3.11}$$

For ζ in Class I, a single interval $\aleph$ extends from $x = 0$ to ∞. In Class III and Class II, the x axis is broken up into two or more open intervals, and we denote these $\aleph_1$, $\aleph_2$, ..., beginning at the right. It is of interest to note that in Class II, the solutions $\vec{\theta}_2$ and $\vec{\theta}_3$ become "identical" at

x* in the sense that the eigenvectors of $\underset{\sim}{\Phi}_0$ (see Appendix A) corresponding to μ_2 and μ_3 become identical, as, of course, do the eigenvalues themselves. Similarly in Class III, $\vec{\theta}_1$ and $\vec{\theta}_2$ become identical at x*.

4. ASYMPTOTIC EVALUATION OF $\vec{\theta}$

The desired solution $\vec{\theta}$ is defined by the boundedness condition, Eq. (2.7c). For large x, the behavior of the solutions of the differential equation (2.7b) was shown previously[3] to be exponential growth or decay, the coefficients of x in the exponentials being just the eigenvalues of the coefficient matrix, evaluated at $x = \infty$. Moreover, for $\mathrm{Re}(\tau)$ positive, it was shown that a single eigenvalue has negative real part.

The formal solutions Eq. (3.3), derived in the last section, behave in the same fashion for large x, for the h_i and k_i integrals become linear in x near the region of chemical equilibrium. Now for large ϵ, the eigenvalue problem at $x = \infty$ has a perturbation solution[8] through a power series in ϵ^{-1},

$$[\epsilon\, \underset{\sim}{\Phi}_0(\infty, \zeta) + \underset{\sim}{\Phi}_1(\infty, \nu) - (\epsilon\mu^{(0)} + \mu^{(1)} + \epsilon^{-1}\mu^{(2)} + \ldots)\underset{\sim}{I}]$$

$$\cdot\, [\vec{\nu}^{(0)} + \epsilon^{-1}\, \vec{\nu}^{(1)} + \ldots] = 0$$

which exists provided that $\underset{\sim}{\Phi}_0(\infty, \zeta)$ has distinct eigenvectors. Then, with the exception of the case of degenerate eigenvectors of $\underset{\sim}{\Phi}_0(\infty, \zeta)$ [viz., $\zeta = \pm\, i(c_o \eta^{\frac{\pm}{2}})_{x=\infty}$ and $\zeta = (u)_{x=\infty}$ which we do not treat directly],

it is seen that the $x \to \infty$ solutions agree with the expressions of the last section when carried to large x. The $\epsilon \to \infty$ limit and the $x \to \infty$ limit are, therefore, interchangeable; and the solution $\vec{\theta}$ can be investigated directly through the $x \to \infty$ behavior of the ϵ-asymptotic solutions.

The validity of the expressions, Eq. (3.3), as asymptotic solutions of the differential equations (2.7b) depends, according to the theory of the parameter problem,[5] only on the behavior of the functions $h_i(x, \zeta)$. It will be convenient in what follows to regard the formal solutions as defined not only on the axis of real values of x but also for complex values z. For ϵ real, then, the region of validity (the admissible region) $\mathcal{K}_i$ of the z-plane for the i^{th} solution depends upon the existence of paths $P_j(z)$ in $\mathcal{K}_i$ for every z such that P_j is of bounded contour length and such that $h_j - h_i$ is, in real part, non-increasing along the path, i.e.,

$$\begin{aligned} &\mathrm{Re}[h_{ji}(z') - h_{ji}(z)] \geq 0 \\ &\qquad h_{ji} = h_j - h_i \end{aligned} \tag{4.1}$$

for all z' on P_j, from an origin z_j' to the point in question z. The existence of such paths for every j is sufficient to prove the admissibility of solution i in $\mathcal{K}_i$.

In order to consider condition (4.1) in connection with $\vec{\theta}_1$, we write

$$h_{21}(z) = \int_0^z \mu_{21}(z')dz'$$

$$h_{31}(z) = h_{41}(z) = \cdots = h_{n+4,1}(z) = \int_0^z \mu_{31}(z')dz' \tag{4.2}$$

$$\mu_{ij} = \mu_i - \mu_j \, .$$

We consider h_{21} and h_{31} along the real axis for the present, restricting attention to an interval $\aleph$ for which $\vec{\theta}_1$, $\vec{\theta}_2$, ... are defined. As long as $\mathrm{Re}(\mu_{21})$ and $\mathrm{Re}(\mu_{31})$ do not change sign, $\mathrm{Re}(h_{21})$ and $\mathrm{Re}(h_{31})$ are monotone in x. If $\mathrm{Re}(h_{i1})$ is monotone non-increasing, then a suitable path P_i originates at the left and extends to increasing values of x. If $\mathrm{Re}(h_{i1})$ is monotone non-decreasing, then a suitable path P_i originates at a large value of x. and extends to the left. In either case, an admissible region $\mathfrak{K}_1$ can be found, which includes that portion of the real axis on which neither $\mathrm{Re}(\mu_{21})$ nor $\mathrm{Re}(\mu_{31})$ vanishes. In view of the interchangeability of the ϵ and x limits, it is clear that such a region can be extended to infinite x.

From Eq. (3.5), we compute

$$\mu_{21} = 2\kappa s/\eta u$$

$$\mu_{31} = (\zeta + \kappa s)/\eta u. \tag{4.3}$$

Now for any ζ, it is seen that $\mathrm{Re}(\mu_{21})$ and $\mathrm{Re}(\mu_{31})$ do not change sign in any interval of definition $\aleph$ of $\vec{\theta}_1$, $\vec{\theta}_2$, ..., for the points where s vanishes are just the endpoints of the intervals for Class III values of ζ.

Similarly, the validity of $\vec{\theta}_2$ is proved by consideration of

$$\mu_{12} = -2\kappa s/\eta u$$

$$\mu_{32} = (\zeta - \kappa s)/\eta u \tag{4.4}$$

whose real parts either vanish identically or do not vanish at all (depending on ζ) on the $\aleph$ intervals.

For ζ in Class I, it follows that the admissible region $\mathcal{K}_1$ includes the entire x axis so that

$$\vec{\theta} \sim \vec{\theta}_1 \quad \text{for all } x. \tag{4.5}$$

For Class II and Class III, however, we have

$$\vec{\theta} \sim \vec{\theta}_1 \quad \text{for } x \text{ on } \aleph_1 \tag{4.6}$$

but are left with the problem of the continuation of $\vec{\theta}$ to the left of the so-called turning points x^*.

There are essentially two techniques used in solving turning-point problems and it seems appropriate to pause to mention some general characteristics of these. The first involves an attempt to proceed around the turning point by analytic continuation into the complex z (independent variable) plane. Ordinarily this process is terminated at certain Stokes lines across which the asymptotic form of the solutions to the differential equations changes abruptly. Usually this approach involves solution of the "connection problem;" that is, it involves the determination of the solutions at the turning point itself by means of an appropriate "stretching transformation."[5] This first approach, although extensively investigated, seemingly has not been developed to any degree of generality, with proofs of its validity being not entirely satisfactory.

A second approach is that of Langer and McKelvey[9-12] which concentrates at the outset on the nature of the equations at the turning point, in much the manner of the solution of the connection problem, but

in such a way as to develop a series which is valid both at the turning point and away from it. The process of "piecing together" solutions is thereby avoided and the proof of asymptotic validity becomes relatively direct.

Now it will not be surprising to find that the nature of the present problem at the turning point depends upon whether ζ is in Class II or Class III and in the latter case on the behavior of $c_o^2\eta$ at x^*. Thus several types of problems involve us here and it will be convenient to employ both approaches to the turning-point problem. Most of the problems encountered here can, in fact, be solved by the first approach, without the necessity of attacking the connection problem at all, while the Langer method seems more direct for the purpose of completing the analysis. The remainder of this section is concerned solely with the first approach and requires no additional analysis beyond the application of the condition, Eq. (4.1).

Class II Values of ζ

For the sake of simplicity, let us suppose that a single point at which $u = \zeta$ exists; it will be evident that the procedure described here applies equally well irrespective of the number of such points. According to Sec. 3, there exist solutions $\vec{\theta}_1$, $\vec{\theta}_2$, ... defined on $\aleph_1(x^* < x)$ and a second set, $\vec{\theta}_1$, $\vec{\theta}_2$, ... defined on $\aleph_2(0 \leq x < x^*)$. Rather than deal with these, however, it is simpler to redefine the $\vec{\theta}_i$ to be the set of functions obtained from the set valid on $\aleph_1$ by analytic continuation

throughout a region $\mathcal{K}$ of the complex z-plane. Now the matrix $\underset{\sim}{T}(z, \zeta)$, the analytic continuation of $\underset{\sim}{T}(x, \zeta)$ to complex z, is differentiable in some strip centered on the x axis, punctured in the neighborhood of x*, as shown in Fig. 1, and in fact is single-valued there. Since $\vec{\theta}_1$, $\vec{\theta}_2$, ... involve only functions which are regular throughout $\mathcal{K}$, and integrals thereof, it follows that as long as $\mathcal{K}$ is simply connected, as in Fig. 1, $\vec{\theta}_1$, $\vec{\theta}_2$, ... are regular and single-valued.

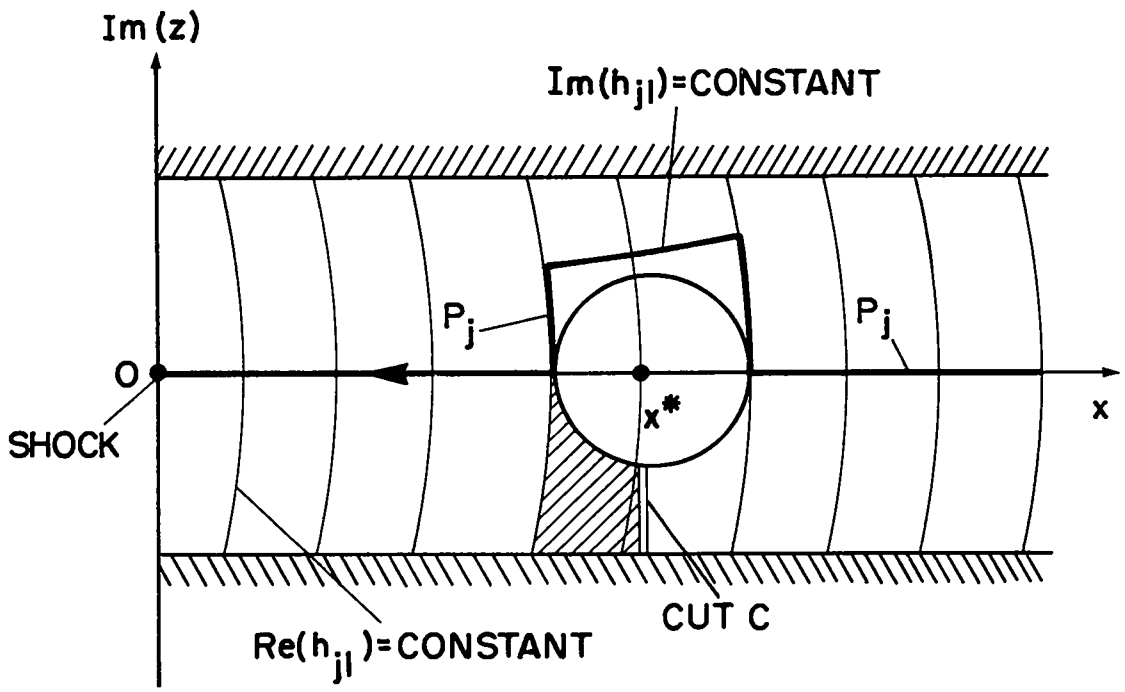

Fig. 1 The region $\mathcal{K}$ of the complex plane through which the series solutions $\vec{\theta}_i$ can be defined by analytic continuation for Class II values of ζ. The turning point x* and its neighborhood are excluded. By virtue of the cut C, $\mathcal{K}$ is simply connected. The light curves are lines of constant $\mathrm{Re}(h_{jl})$ and the paths P_j of the type illustrated (heavy curve) have non-increasing $\mathrm{Re}(h_{jl})$.

We can now investigate condition (4.1) using Eq. (4.3). Since μ_{21} and μ_{31} are real and positive on the real axis, h_{21} and h_{31} are monotonically increasing with x. In region $\mathcal{K}$, then, the lines of constant $\mathrm{Re}(h_{j1})$ are perpendicular to the x axis, as shown in Fig. 1. Therefore paths P_j, originating on the right, can reach all points of $\mathcal{K}$, except the shaded area, simply by proceeding along the x axis and alternately along lines of constant $\mathrm{Re}(h_{j1})$ and $\mathrm{Im}(h_{j1})$ with decreasing $\mathrm{Re}(h_{j1})$, as shown in the figure. Since this argument applies for both $j = 2$ and 3, it follows that $\vec{\theta}_1$ is admissible throughout $\mathcal{K}$, except in the neighborhood of the cut. Thus we conclude

$$\vec{\theta} \sim \vec{\theta}_1 \qquad \text{for all } x \neq x^*. \tag{4.7}$$

Class III Values of ζ

Turning points where $c^2\eta$ increases

In this case, we begin by considering the case of a turning point through which $c_o^2\eta$ increases, although the case in which it decreases is related by a simple sign transformation of the independent variable. These cases in which $c_o^2\eta$ is not an extremum at x* can be reduced to an application of a minor generalization of the "singular turning-point problem" [13] for second-order differential equations, the generalization being required by the increased number of equations, i.e., n + 4 (rather than 2) equations.

As for Class II values of ζ, we begin by generalizing the intervals of definition of the series solutions to the complex z-plane. Now,

however, the point x^* is a branch point of the z-plane analytic continuation of the square root $s(x, \zeta)$, whence x^* is also a branch point of μ_1 and μ_2. Analytic continuation of $\vec{\theta}_1$ and $\vec{\theta}_2$ will yield results which depend upon the path of continuation and some care must be exercised with regard to notation.

Begin, then, with the functions $\vec{\theta}_1$, $\vec{\theta}_2$, $\vec{\theta}_3$, ... , defined in Sec. 3, on the interval $\aleph_1$ and compute $\mu_{21}(z)$ and $\mu_{31}(z)$ in the neighborhood of x^*,

$$\mu_{21}(z) = [2\kappa d^{\frac{1}{2}}/\eta u]_{x^*}(z - x^*)^{\frac{1}{2}}[1 + O(z - x^*)]$$

$$\mu_{31}(z) = [i/\eta^{\frac{1}{2}}\kappa]_{x^*}[1 + O(z - x^*)] \qquad (4.8)$$

where

$$d = d(c_o^2\eta)/dx,$$

and where we have taken ζ to lie on the upper imaginary axis. We need not consider the conjugate points at all, since roots of $V(\tau, \epsilon)$ occur in conjugate pairs, as is proved in Appendix B. It follows from Eq. (4.8) that for $z \approx x^*$,

$$h_{21}(z) - h^*_{21} = [4\kappa d^{\frac{1}{2}}/3\eta u]_{x^*}(z - x^*)^{3/2} + \ldots$$

$$h_{31}(z) - h^*_{31} = [i/\eta^{\frac{1}{2}}\kappa]_{x^*}(z - x^*) + \ldots \qquad (4.9)$$

$$h^*_{ij} = h_{ij}(x^*) .$$

The loci,

$$\mathrm{Re}[h_{21}(z) - h^*_{21}] = 0$$

$$\mathrm{Re}[h_{31}(z) - h^*_{31}] = 0 \qquad (4.10)$$

are referred to as <u>transition</u> lines, whose significance will be evident in what follows. Near x^*, we see that these are radial lines emanating from x^*, viz.,

$$\varphi = \arg(z - x^*)$$

$$\varphi_{21} = \pm \pi/3, \pm \pi, \pm 5\pi/3, \ldots \tag{4.11}$$

$$\varphi_{31} = 0, \pm \pi$$

where the subscripts classify these values of φ in accordance with the h_{21} or the h_{31} condition. Note that the line $\varphi_{31} = \pm \pi$ and the $\varphi_{21} = \pm \pi, \pm 3\pi, \ldots$ lines are exact transition lines, while the others hold only in the limit $z \to x^*$.

Now the solution $\vec{\theta}_1$, which is defined and whose validity has been established for x on $\aleph_1$, presumably will retain its validity in the z-plane near $\aleph_1$. To examine to what extent this is true, we refer to Fig. 2 which shows the transition lines for φ_{21} and the sign of $\mathrm{Re}(h_{21} - h_{21}^*)$ for the neighborhood of x^* and $-\pi < \varphi < \pi$. It is observed that $\mathrm{Re}(h_{21})$ diminishes on paths originating at the right and these paths can be extended outside the sector $-\pi/3 < \varphi < \pi/3$, to include the entire plane with the exception of the axis, $\varphi = \pm \pi$, by employing paths of constant $\mathrm{Re}(h_{21})$ as shown in the figure. The axis is excluded by virtue of the fact that $\vec{\theta}_1$ is singular at $s = 0$ and hence no path can be extended through the turning point.

To proceed with the description of the asymptotic solutions of the differential equations, we now introduce some additional notation. We

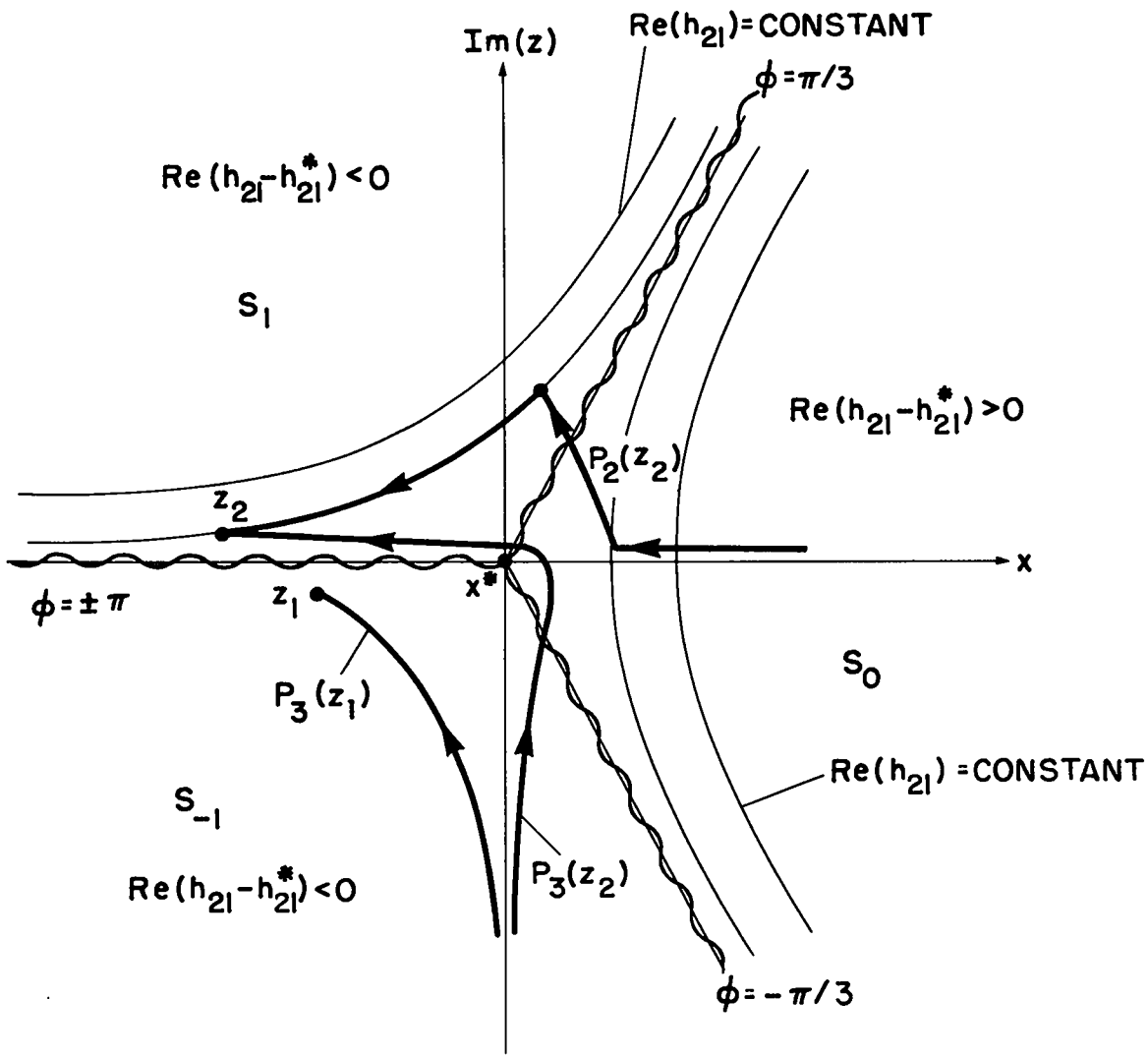

Fig. 2 Paths P_2 in the complex z-plane on which $\mathrm{Re}(h_{21})$ diminishes and P_3 on which $\mathrm{Re}(h_{31})$ diminishes for asymptotic solution $\vec{\theta}_1$, defined by analytic continuation from the real axis $x > x^*$ to points with $|\varphi| < \pi$, $[\varphi = \arg(z - x^*)]$. Points z_1 and z_2 on opposite sides of the slit at $\varphi = \pm \pi$ both lie on such paths, although $P_2(z_2)$ is not shown.

define "sectors" S_i in the $(z - x^*)$-plane by means of the transition lines; near x^* these approach the sectors

$$\begin{aligned} S_0 &: -\pi/3 < \varphi < \pi/3 \\ S_1 &: \pi/3 < \varphi < \pi \\ S_{-1} &: -\pi < \varphi < -\pi/3 \\ S_2 &: \pi < \varphi < 5\pi/3 \\ &\vdots \end{aligned} \tag{4.12}$$

If we denote the analytic continuation of solution $\vec{\theta}_j$ to sector S_i by $\vec{\theta}_j^{(i)}$, then our discussion in the last paragraph proves that $\vec{\theta}_1^{(0)}$, $\vec{\theta}_1^{(1)}$, $\vec{\theta}_1^{(-1)}$ form a solution, which we denote simply $\vec{\theta}^{(0)}$, i.e., by its central sector, asymptotically admissible, with respect to condition (4.1) for h_{21}, in the plane slit at $\varphi = \pm\pi$. We refer to the latter as the Stokes lines for $\vec{\theta}^{(0)}$, since the continuation of $\vec{\theta}^{(0)}$ across them has not been shown to be valid (and, in fact, is not valid).

Similar considerations can be applied to the solution $\vec{\theta}_2$ for we have near x^*,

$$\begin{aligned} h_{12}(z) - h_{12}^* &= -\left[4\kappa d^{\frac{1}{2}}/3\eta u\right]_{x^*}(z - x^*)^{3/2} + \cdots \\ h_{32}(z) - h_{32}^* &= \left[i/\eta^{\frac{1}{2}}\kappa\right]_{x^*}(z - x^*) + \cdots \end{aligned} \tag{4.13}$$

yielding precisely the same set of transition lines as for $\vec{\theta}_1$. In Fig. 3 are shown the transition lines for h_{12} on $-\pi/3 < \varphi < 5\pi/3$ and the sign of $\mathrm{Re}(h_{12} - h_{12}^*)$ is shown in the sectors S_0, S_1, and S_2. Paths of

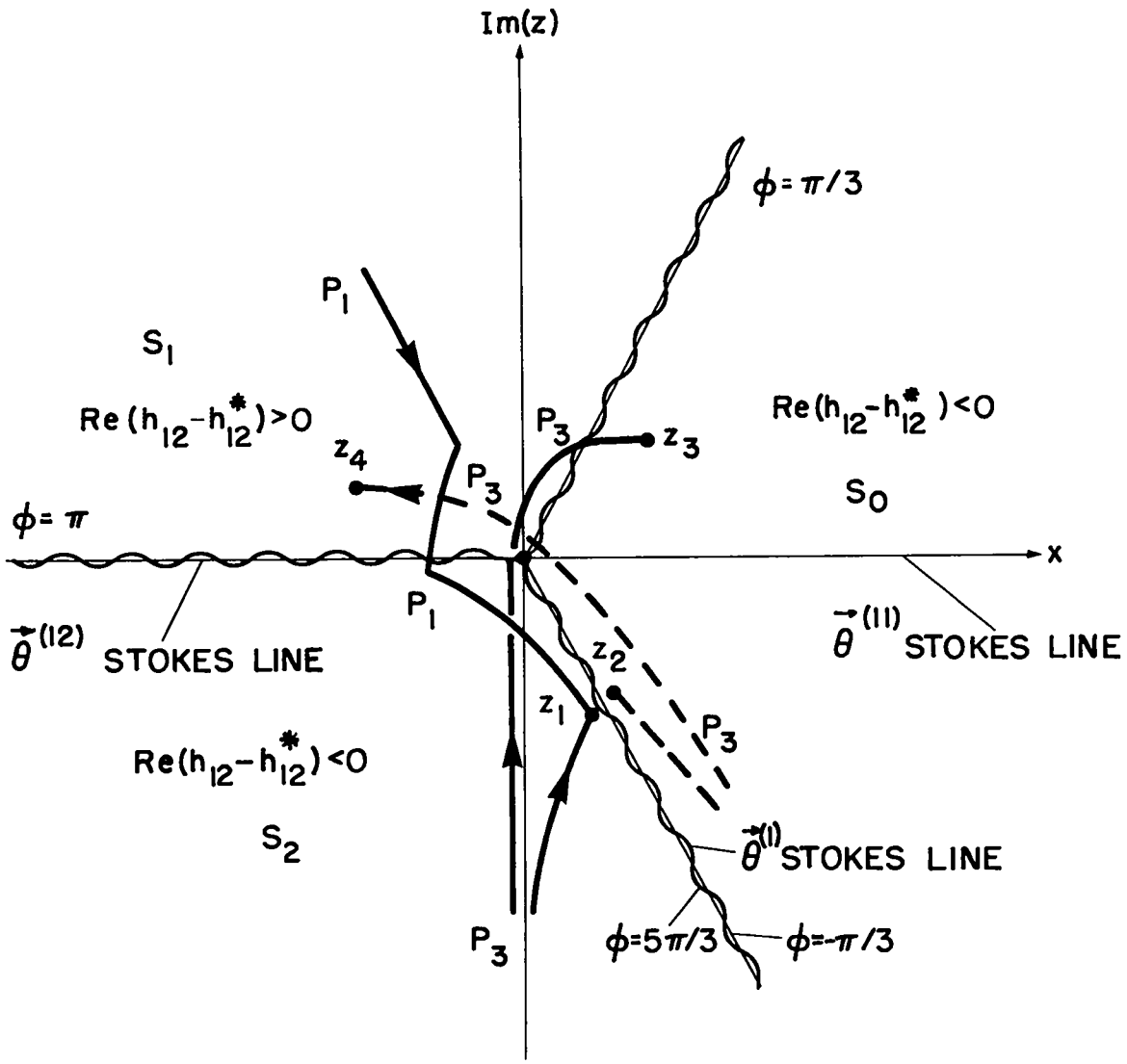

Fig. 3 Paths P_1 in the complex z-plane on which $Re(h_{12})$ diminishes and P_3 on which $Re(h_{32})$ diminishes for asymptotic solution $\vec{\theta}^{(1)}$ defined by analytic continuation of $\vec{\theta}_2$ from the real axis $x > x^*$ to points with $-\pi/3 < \varphi < 5\pi/3$. Points z_1 and z_2 on opposite sides of the slit both lie on P_1 paths (that for z_2 is not shown) but two types of P_3 paths are required. The dashed P_3 paths cannot enter sector S_2, while the solid P_3 paths cannot enter the $\varphi \leq 0$ region.

decreasing $\mathrm{Re}(h_{12})$ then originate in sector S_1 and cover the plane slit at $\varphi = -\pi/3, 5\pi/3$. The solutions $\vec{\theta}_2^{(1)}$, $\vec{\theta}_2^{(2)}$, $\vec{\theta}_2^{(0)}$, denoted simply $\vec{\theta}^{(1)}$, are, therefore, admissible with respect to condition (4.1) for h_{12}, and have Stokes lines at $\varphi = -\pi/3, 5\pi/3$.

These considerations can be applied to the continuation of the $\vec{\theta}_1$ and $\vec{\theta}_2$ series into other sectors to establish a collection of solutions which are admissible on certain slit-planes, as seen in Table I, where again condition (4.1) has been applied only between h_1 and h_2. Although this list could be extended indefinitely, it is readily seen that, at each point z, only two distinct solutions exist. Thus $\vec{\theta}_1^{(i)}$ and $\vec{\theta}_2^{(i\pm3)}$ differ by a constant factor, so that Table I contains but three distinct solutions, say $\vec{\theta}^{(0)}$, $\vec{\theta}^{(1)}$, and $\vec{\theta}^{(-1)}$, although solutions $\vec{\theta}^{(2)}$ and $\vec{\theta}^{(-2)}$ will also prove useful.

TABLE I

System of asymptotic solutions of differential Eq. (2.7b), admissible with respect to condition (4.1) for (i, j) = 1, 2, near a turning point x^* at which $c_o^2\eta$ is increasing.

Solution	Definition	Stokes lines $\arg(z - x^*)$
$\vec{\theta}^{(0)}$	$\vec{\theta}_1^{(0)}$, $\vec{\theta}_1^{(1)}$, $\vec{\theta}_1^{(-1)}$	$\pm\ \pi$
$\vec{\theta}^{(1)}$	$\vec{\theta}_2^{(1)}$, $\vec{\theta}_2^{(2)}$, $\vec{\theta}_2^{(0)}$	$-\ \pi/3,\quad 5\pi/3$
$\vec{\theta}^{(-1)}$	$\vec{\theta}_2^{(-1)}$, $\vec{\theta}_2^{(-2)}$, $\vec{\theta}_2^{(0)}$	$-\ 5\pi/3,\quad \pi/3$
$\vec{\theta}^{(2)}$	$\vec{\theta}_1^{(2)}$, $\vec{\theta}_1^{(3)}$, $\vec{\theta}_1^{(1)}$	$\pi/3,\quad 7\pi/3$
$\vec{\theta}^{(-2)}$	$\vec{\theta}_1^{(-2)}$, $\vec{\theta}_1^{(-3)}$, $\vec{\theta}_1^{(-1)}$	$-\ 7\pi/3,\ -\ \pi/3$

It is of interest to note that in the central sector of the plane slit by the Stokes lines, the solution is recessive but is dominant in its outer sectors. For example in S_0, $\vec{\theta}^{(0)}$ is recessive, since $h_{21} - h_{21}^*$ has positive real part and $\vec{\theta}_2^{(0)}$ grows in magnitude relative to $\vec{\theta}_1^{(0)}$ as ϵ increases. In S_1, however, $\vec{\theta}_2^{(1)}$ is recessive. In fact, it is just this property of the central sector which is used in establishing the condition (4.1).

Turning now to the validity of this condition for $j = 3$, we employ the second of Eq. (4.9) and (4.13) from which it is seen that P_3 paths must proceed in the upward direction in the z-plane. For $\vec{\theta}^{(0)}$, it is seen from Fig. 2 that such paths exist for all points in the region previously found to be admissible with respect to the h_{21} condition. Similarly for $\vec{\theta}^{(-1)}$ which has Stokes lines at $\varphi = \pi/3, -5\pi/3$, the slit-plane is entirely covered by P_3 paths. For $\vec{\theta}^{(1)}$, however, the Stokes lines extend downward, as in Fig. 3, so that for points with $\mathrm{Im}(z) \leq 0$, the P_3 paths must originate on the same side of the Stokes line. Thus the h_3 condition splits this solution into two portions:

$$\vec{\theta}^{(11)} \text{ valid in } \quad 0 < \varphi < 5\pi/3$$

$$\vec{\theta}^{(12)} \text{ valid in } \quad -\pi/3 < \varphi < \pi. \qquad (4.14)$$

Since $\vec{\theta}^{(-2)}$ differs from $\vec{\theta}^{(1)}$ by a factor, a similar splitting is imposed on it.

Turning points where $c_o^2\eta$ decreases

For turning points at which $c_o^2\eta$ decreases, the solutions and their Stokes lines are somewhat altered. It is straightforward to apply the above methods to obtain the corresponding solutions. We begin with $\vec{\theta}_1$, $\vec{\theta}_2$, ... , not on $\aleph_1$, but to the left of x* and proceed by analytic continuation as before. Thus, the first of Eq. (4.9) becomes

$$h_{21}(z) - h_{21}^* = [4\kappa(-d)^{\frac{1}{2}}/3\eta u]_{x^*}(x^* - z)^{3/2} + \ldots \qquad (4.15)$$

Defining sectors S_0, S_1, ... by the transition lines which near x* are given by

$$\tilde{\varphi} = \arg(x^* - z)$$

$$\tilde{\varphi}_{21} = \pm \pi/3, \pm \pi, \ldots$$

$$\tilde{\varphi}_{31} = 0, \pm \pi$$

as indicated in Fig. 4, we can readily obtain the system of solutions in Table II. The regions of validity refer, as in Table I, only to the condition (4.1) applied between $\vec{\theta}_1$ and $\vec{\theta}_2$. Note that $\vec{\theta}_2$ is now recessive in S_0.

Imposing the condition (4.1) for j = 3 leads again to P_3 paths directed upward in the z-plane, whence $\vec{\theta}^{(-1)}$ and $\vec{\theta}^{(2)}$ are seen, from Fig. 4, to be split into two parts, for example:

$$\vec{\theta}^{(-11)} \quad \text{valid in} \quad -5\pi/3 < \tilde{\varphi} < 0$$

$$\vec{\theta}^{(-12)} \quad \text{valid in} \quad -\pi < \tilde{\varphi} < \pi/3. \qquad (4.16)$$

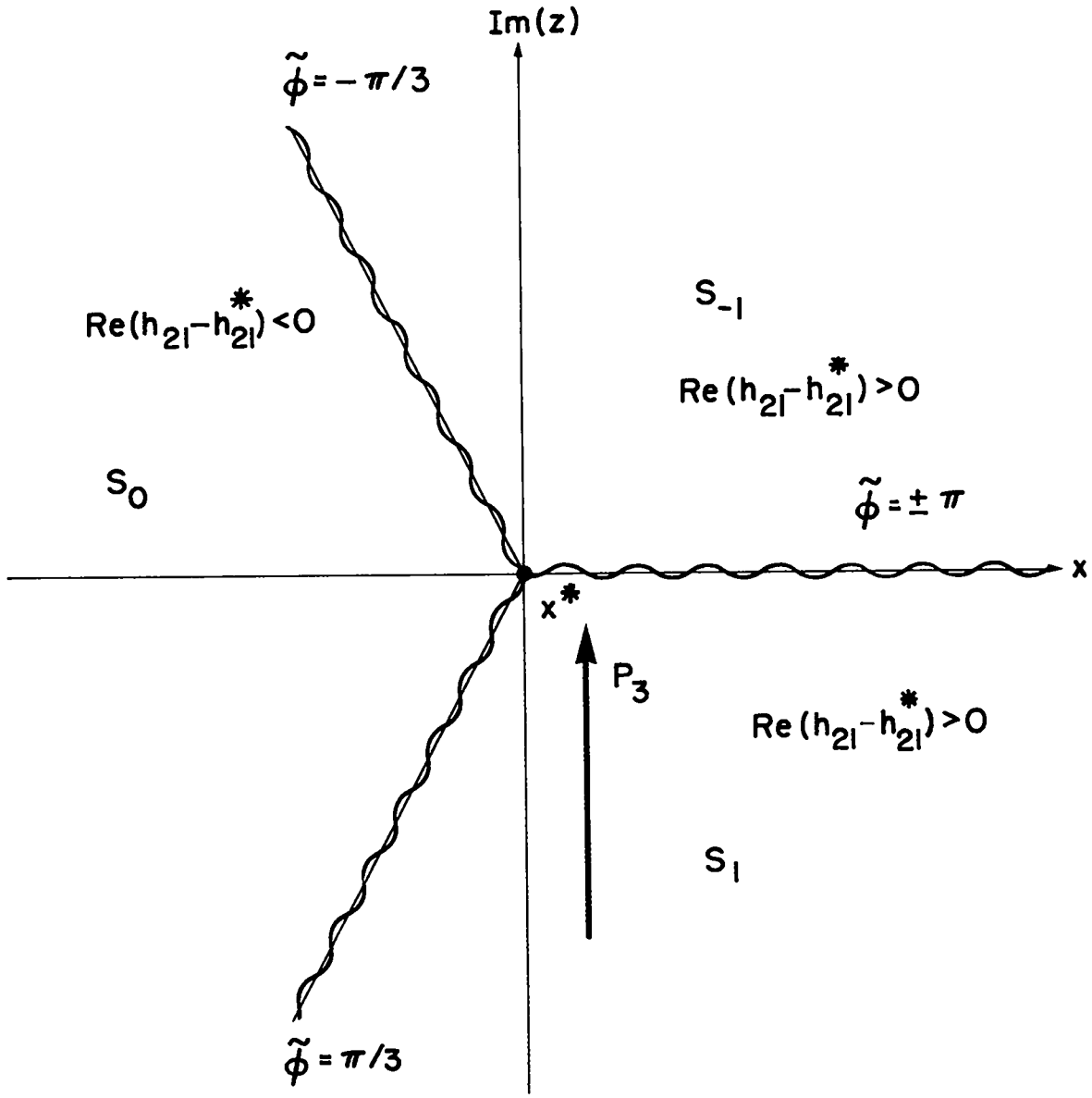

Fig. 4 Definition of sectors S_0, S_1, and S_{-1} for a turning point x^* through which $c_o^2\eta$ decreases. The sign of $Re[h_{21} - h_{21}(x^*)]$ obtained from the analytic continuation of $\vec{\theta}_1$ and $\vec{\theta}_2$ from the real axis $x < x^*$ is indicated. P_3 paths on which condition (4.1) is valid proceed upward in the z-plane, as indicated.

TABLE II

System of asymptotic solutions of differential Eq. (2.2), admissible with respect to condition (4.1) for (i, j) = 1, 2, near a turning point x* at which $c_o^2\eta$ is decreasing.

Solution	Definition	Stokes lines arg(x* - z)
$\vec{\theta}(0)$	$\vec{\theta}_2(0)$, $\vec{\theta}_2(1)$, $\vec{\theta}_2(-1)$	$\pm\ \pi$
$\vec{\theta}(1)$	$\vec{\theta}_1(1)$, $\vec{\theta}_1(2)$, $\vec{\theta}_1(0)$	$-\ \pi/3,\quad 5\pi/3$
$\vec{\theta}(1)$	$\vec{\theta}_1(-1)$, $\vec{\theta}_1(-2)$, $\vec{\theta}_1(0)$	$-\ 5\pi/3,\quad \pi/3$
$\vec{\theta}(2)$	$\vec{\theta}_2(2)$, $\vec{\theta}_2(3)$, $\vec{\theta}_2(1)$	$\pi/3,\quad 7\pi/3$
$\vec{\theta}(-2)$	$\vec{\theta}_2(-2)$, $\vec{\theta}_2(-3)$, $\vec{\theta}_2(-1)$	$-\ 7\pi/3,\quad -\ \pi/3$

Continuation problem

The continuation of the asymptotic expression for $\vec{\theta}$ beyond a turning point divides into two problems, then, depending upon whether $c_o^2\eta$ is increasing or decreasing at x*; and a complete determination of $\vec{\theta}$ for all x will depend upon the configuration of turning points along the x axis. It is convenient to carry out the determination of $\vec{\theta}$ under the assumption that $c_o^2\eta$ has some simple form, although more complicated forms can be treated with little additional difficulty. Three profiles will be considered, as shown in Fig. 5; each occurs for certain values of the

parameters for the idealized, one-reaction detonations whose stability has been studied numerically.[4] Profile I designates those steady detonations in which $c_o^2\eta$ increases monotonically; profile D, those in which $c_o^2\eta$ decreases monotonically; and profile M designates those in which $c_o^2\eta$ has a single maximum as a function of x.

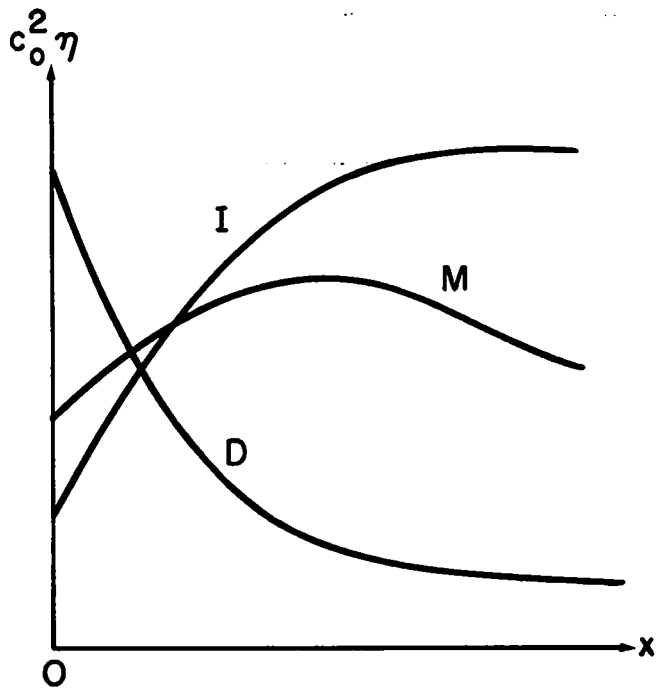

Fig. 5 Profiles of $c_o^2\eta$ in the steady flow which are considered. Profile M includes both cases with regard to the relative values of $c_o^2\eta$ at $x = 0$ and $x = \infty$.

Profile I. For detonations having profile I behavior, we first note that (for ζ in Class III) to the right of x*, i.e., on interval $\aleph_1$, we have $\vec{\theta} \sim \vec{\theta}_1$, Eq. (4.6), and $c_o^2\eta$ increases at x*. The asymptotic expressions of Table I, as modified by Eq. (4.14), are directly applicable. Thus $\vec{\theta}_1$ is contained in $\vec{\theta}^{(0)}$ which breaks down at $\varphi = \pm \pi$. To solve the continuation problem, we write $\vec{\theta}$ as a linear combination of two independent solutions, valid on $\varphi = \pi$ [see Table I and Eq. (4.14)]

$$\vec{\theta} = c_1\vec{\theta}^{(11)} + d_1\vec{\theta}^{(2)} \tag{4.17}$$

and on $\varphi = -\pi$

$$\vec{\theta} = c_2\vec{\theta}^{(-1)} + d_2\vec{\theta}^{(-21)}. \tag{4.18}$$

Contributions from the remaining n + 2 solutions need not be included, for reasons which will be given later. Now in S_1, $\vec{\theta}^{(0)}$ and Eq. (4.17) are valid. Since $\vec{\theta}^{(11)}$ and $\vec{\theta}^{(2)}$ are identical, viz. $\vec{\theta}_1^{(1)}$, in S_1 and $\vec{\theta}^{(11)}$ is recessive there, it follows that $d_1 = 1$. Similar considerations in S_{-1} prove that $d_2 = 1$.

The remaining coefficients are determined by the condition that $\vec{\theta}$ is single-valued. Equating Eq. (4.17) and (4.18) for $x < x^*$ and utilizing the fact that $\vec{\theta}^{(-1)}$ and $\vec{\theta}^{(2)}$ differ by a constant factor, as do $\vec{\theta}^{(11)}$ and $\vec{\theta}^{(-21)}$, we see that

$$\vec{\theta} \sim \vec{\theta}^{(-21)} + \vec{\theta}^{(2)} = \vec{\theta}_1^{(-1)} + \vec{\theta}_1^{(11)}. \tag{4.19}$$

That is, $\vec{\theta}$ is obtained by adding the analytic continuations of $\vec{\theta}_1$ via both the upper and the lower half-planes.

The absence of the n + 2 other solutions from Eq. (4.17) and (4.18) is justified by the consideration of $\vec{\theta}$ in S_2 and S_{-1}, respectively. Since, for these z, h_{31} and h_{32} have larger real parts than at x*, any contribution of a μ_3-type solution would be dominant over the μ_1- and μ_2-type solutions. Since $\vec{\theta}$ itself is known asymptotically in S_{-1}, viz., $\vec{\theta}_1^{(-1)}$, it follows by single-valuedness that μ_3-type contributions are not permitted.

It can be readily seen that $\vec{\theta}_1^{(1)}$ contains for the square root s, for $x < x^*$, $s = i\,|s|$ and hence is a μ_1-type solution, while $\vec{\theta}_1^{(-1)}$ has $s = -i\,|s|$ and hence is a μ_2-type solution. To express $\vec{\theta}$ in most convenient form, we now specify $\vec{\theta}_1$ and $\vec{\theta}_2$ completely (to highest order) by specifying the lower limit of integration in Eq. (3.6) and (3.10) to be $x_o = 0$. The k_i integrals then exist for all $x \neq x^*$ and continue to have derivatives E_{ii}, provided the integration path for $x > x^*$ avoids the turning point by a small excursion into the upper half z-plane. With this understanding, then,

$$\vec{\theta}^{(1)} = \vec{\theta}_1$$

$$\vec{\theta}_1^{(-1)} = \alpha\vec{\theta}_2 \qquad (4.20)$$

$$\vec{\theta} \sim \vec{\theta}_1 + \alpha\vec{\theta}_2, \text{ for } x < x^*$$

with the coefficient α found to be

$$\alpha(\epsilon, \zeta, \upsilon) = \exp \beta(\epsilon, \zeta, \upsilon)$$

$$\beta(\epsilon, \zeta, \upsilon) = \oint_C [\epsilon\mu_1 + E_{11}]dz \qquad (4.21)$$

where C is the contour enclosing x* shown in Fig. 6.

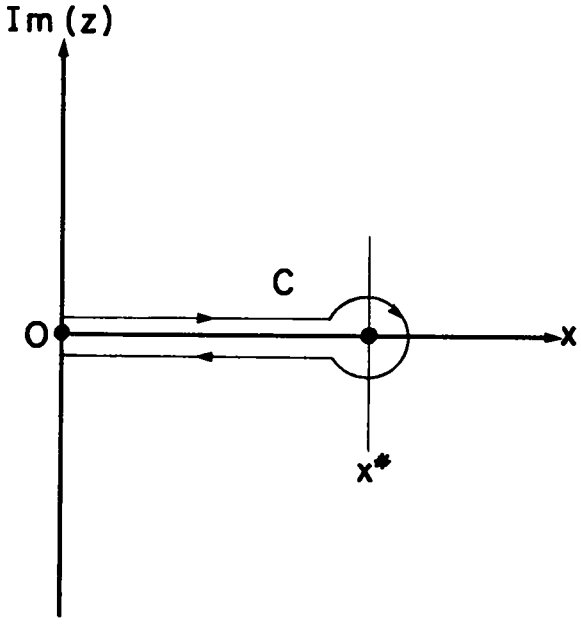

Fig. 6 Contour C in the complex z-plane used for the definition of $\alpha(\epsilon, \zeta, \upsilon)$, Eq. (4.21), required for the continuation problem at a turning point x* at which $c_o^2\eta$ is increasing with distance from the shock.

Profile D. For Class III values of ζ, $c_o^2\eta$ decreases at the turning point. The asymptotic expressions of Table II, modified by Eq. (4.16) are now applicable. For $x > x^*$, we had by Eq. (4.6), $\vec{\theta} \sim \vec{\theta}_1$. Now the entry in Table II which is valid for $x > x^*$ and of μ_1-type is $\vec{\theta}_1^{(1)}$, as is readily verified by consideration of μ_1 in the neighborhood of x^*. Now $\vec{\theta}_1^{(1)}$ is contained in $\vec{\theta}^{(1)}$ which is valid for $x < x^*$ as well, i.e., for $\tilde{\varphi} = 0$. Thus for profile D,

$$\vec{\theta} \sim \begin{cases} \vec{\theta}_1^{(0)} & \text{for } x < x^* \\ \vec{\theta}_1^{(1)} & \text{for } x > x^*. \end{cases}$$

If we now utilize definitions of $\vec{\theta}_1$ and $\vec{\theta}_2$ analogous to those for profile I, viz., $x_o = 0$ in Eq. (3.6) and (3.10), with the integration paths for h_1, h_2, k_1, and k_2 avoiding x^* by a lower half z-plane excursion, this can be written simply as

$$\vec{\theta} \sim \vec{\theta}_1 \text{ for all } x \neq x^*. \tag{4.22}$$

Profile M. To treat profile M, we consider the value of $\zeta = i\,(c_o\eta^{\frac{1}{2}})_{max}$ separately, for the turning point in that case apparently differs from those we have already considered. We return to its study in Sec. 6. For all other Class III values of ζ, we simply combine the results for profile I and profile D. We denote by x_1^* the turning point, if any, where $c_o^2\eta$ is decreasing and simply use x^* to denote the point, if any, at which $c_o^2\eta$ is increasing. For those ζ for which only one turning point exists, the considerations of profile I or D apply. For those ζ for which two turning points exist, the outer one x_1^* is of the

profile D type. The continuation problem there yields

$$\vec{\theta} \sim \vec{\theta} \text{ for } x > x^*,\ x \neq x_1^* \tag{4.23}$$

where $\vec{\theta}_1$ and $\vec{\theta}_2$ are defined as for profiles I and D, i.e., $x_o = 0$, and the h_i, k_i integration paths excise x^* via the upper half-plane and x_1^* via the lower half-plane. The continuation problem at x^* is therefore typical of profile I, and we obtain

$$\vec{\theta} \sim \vec{\theta}_1 + \alpha\vec{\theta}_2, \quad \text{for } x < x^* \tag{4.24}$$

with α given in Eq. (4.21) and with contour C encircling x^* but not x_1^*.

5. ASYMPTOTIC EVALUATION OF $V(\tau, \epsilon)$

The asymptotic evaluation of $V(\tau, \epsilon)$ requires, according to Eq. (2.7a), the determination of the function $L(\epsilon, \zeta, \upsilon)$ which to highest order in ϵ is

$$L(\epsilon, \zeta, \upsilon) = \zeta b_1 + ib_2 - \vec{\theta}(0, \zeta, \upsilon, \epsilon) \cdot (\zeta\vec{h}_t + i\vec{h}_y). \tag{5.1}$$

The evaluation of b_1 and b_2 will evidently be the major task of this section, since the scalar product is essentially known from our expressions for $\vec{\theta}$.

ζ in Class I

Here we distinguish between those ζ for which $h_1(x, \zeta)$ is pure imaginary and those for which it has a real part. The former, $\mathrm{Re}(\zeta) = 0$, $\mathrm{Im}(\zeta) > (c_o\eta^{\frac{1}{2}})_{max}$, we denote as Class Ia; and the latter, $\mathrm{Re}(\zeta) = 0$, $\mathrm{Im}(\zeta) < (c_o\eta^{\frac{1}{2}})_{min}$, or $\mathrm{Re}(\zeta) > 0$ but ζ not in Class II, we designate as

Class Ib. Now the integrals b_1 and b_2 have the asymptotic form

$$b_1 \sim \int_0^\infty \Delta(x, \zeta, \upsilon) \exp [\epsilon h_1(x, \zeta)]dx$$

$$\Delta(x, \zeta, \upsilon) = \exp [k_1(x, \zeta, \upsilon)] [\underset{\sim}{T}(x, \zeta) \cdot \hat{e}_1] \cdot \underset{\sim}{A}_x^{-1} \cdot \vec{g}_t \qquad (5.2)$$

with h_1 and Δ regular functions of x. For Class Ia, h_1 is pure imaginary and

$$|h_1| = \int_0^x i\mu_1(x', \zeta)dx'$$

increases monotonically with x. Thus, we can transform to $\hat{z} = |h_1|$ as integration variable to obtain a Fourier-type integral, viz.,

$$b_1 \sim \int_0^\infty e^{-i\epsilon\hat{z}} \Delta(x, \zeta, \upsilon)[i\mu_1(x, \zeta)]^{-1}d\hat{z} .$$

Since $\vec{g}_t$ is proportional to the chemical rate (see Ref. 3) which vanishes exponentially with x, as $x \to \infty$, and since $\hat{z}$ is linear in x for large x, it follows that Δ and all its derivatives with respect to $\hat{z}$ vanish at $\hat{z} = \infty$. Thus b_1 can be evaluated asymptotically[14] in ϵ to satisfy the order relation

$$b_1 = O(1/\epsilon) . \qquad (5.3a)$$

Identical considerations show also that

$$b_2 = O(1/\epsilon) . \qquad (5.3b)$$

For Class Ib, h_1 has a real part which is negative and decreases linearly with x as $x \to \infty$. Thus, Eq. (5.2) yields a Laplace-type

integral,†

$$|b_1| \leq \int_0^\infty e^{-\epsilon\hat{z}} \; |\Delta(x, \zeta, \upsilon)| \; [-\mathrm{Re}(\mu_1)]^{-1} d\hat{z}$$

$$\hat{z}(x, \zeta) = -\mathrm{Re}[h_1(x, \zeta)] \; .$$

Since $|\Delta| \; [-\mathrm{Re}(\mu_1)]^{-1}$ is bounded (say, by M), it follows that

$$|b_1| \leq M \int_0^\infty e^{-\epsilon\hat{z}} dz = O(1/\epsilon) \; . \tag{5.4}$$

The same order relation is satisfied, of course, by b_2.

ζ in Class II

For those (real) ζ in Class II, $\vec{\theta} \sim \vec{\theta}_1$ remains valid except in the neighborhood of the turning points x_i^*. To evaluate b_1 and b_2 for this case, the path of integration can be deformed into the upper half z-plane so as to excise the turning points, without altering the values of b_1 and b_2. Along such a path K, $\vec{\theta} \sim \vec{\theta}_1$ is valid, and we have to highest order

$$b_1 \sim \int_K \exp\,[\epsilon h_1(x, \zeta)] \; \Delta(x, \zeta, \upsilon) dx,$$

as in Eq. (5.2); K extends to $x = \infty$, of course. It is seen from the expression for E_{11} in Appendix A that the integrand is regular at the

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† The symbol $\hat{z}$ is used repeatedly within this section as a variable of integration, but its definition varies with each usage.

turning points (although correction terms in $\vec{\theta}_1$ might be singular there), and the path K can be replaced by the real axis once more. Just as for ζ in Class Ib, then,

$$b_1 = O(1/\epsilon)$$
$$b_2 = O(1/\epsilon). \tag{5.5}$$

ζ in Class III

The discussion in Class III becomes considerably more complicated by virtue of the singularities in $\vec{\theta}_1$ and $\vec{\theta}_2$ at the turning point. As a preliminary to our discussion, it is useful to first write these asymptotic expressions $\vec{\theta}_1$ and $\vec{\theta}_2$ so that the infinity associated with x^* is evident. From the expressions for E_{11} and E_{22} (which determine k_1 and k_2) in Appendix A, it is seen that, for turning points at which $c_o^2\eta$ is not an extremum, k_1 and k_2 are infinite at x^* only in the contribution from the $-\frac{1}{2}d\ \ell n\ s/dx$ term, Eq. (A.16); the $1/s$ terms lead to finite contributions. Thus we write

$$k_i(x, \zeta, \upsilon) = -\tfrac{1}{2}\ \ell n\ \frac{s(x, \zeta)}{s(0, \zeta)} + k_i^*(x, \zeta, \upsilon)$$
$$k_i^*(x, \zeta, \upsilon) = \int_0^x [E_{11} + \tfrac{1}{2}d\ \ell n\ s/dx']dx' \tag{5.6}$$

and, using subscript + to denote evaluation behind the shock, we write

$$\vec{\theta}_i(x) = (\underset{\sim}{T} \cdot \hat{e}_i)(s_+/s)^{\frac{1}{2}} \exp\ [\epsilon h_i + k_i^*] .$$

Before considering the specific evaluation of the b integrals, it is profitable to make some general observations concerning them. The contribution to the b's from the neighborhood of the turning point will require special attention, for the asymptotic expressions of the last section are singular at a turning point and are not valid in its neighborhood. The method of evaluation is that introduced for Class II values of ζ; the path of integration is deformed to bypass the turning points without affecting the values of the integral. A certain δ-neighborhood can be avoided by writing, in schematic notation,

$$b = \int_0^{x^*-\delta} I(x)dx + i\delta \int_\pi^0 I(x^* + \delta e^{i\varphi}) e^{i\varphi} d\varphi + \int_{x^*+\delta}^{\infty} I(x)dx \ . \tag{5.7}$$

The integrand $I(x)$ is evaluated then from the asymptotic formulas and is, of course, singular only at x^*. Thus, the result for b will be independent of δ and we are free to employ the $\delta \to 0$ limit without regard to the fact that the asymptotic expression for $\vec{\theta}$ loses its validity near x^*.

Profile I

To evaluate b_1 for profile I, we consider four contributions. First from the (0, x^*) interval, we have, in view of Eq. (4.20), contributions

$$b_{11} = \int_0^{x^*} \vec{\theta}_1 \cdot \underset{\sim}{A}_x^{-1} \cdot \vec{g}_t dx$$

$$b_{12} = \int_0^{x^*} \vec{\theta}_2 \cdot \underset{\sim}{A}_x^{-1} \cdot \vec{g}_t dx \ . \tag{5.8}$$

Now μ_1 and μ_2 are pure imaginary on this interval and the branch points of $\vec{\theta}_1$ and $\vec{\theta}_2$ at x^* can be factored by a change of integration variable. Thus, we introduce a real variable

$$\hat{z} = - is$$

so that Eq. (5.8) becomes

$$b_{11} = \int_0^{\hat{z}_+} \exp\,[i\epsilon\varphi_1(\hat{z})]\ \hat{z}^{\frac{1}{2}}\Delta_1(\hat{z})d\hat{z}$$

$$b_{12} = \int_0^{\hat{z}_+} \exp\,[i\epsilon\varphi_2(\hat{z})]\ \hat{z}^{\frac{1}{2}}\Delta_2(\hat{z})d\hat{z} \qquad (5.9)$$

$$\varphi_i(\hat{z}) = \mathrm{Im}\int_0^x \mu_i dx = \mathrm{Im}\int_{\hat{z}}^{\hat{z}_+} \frac{2\hat{z}\mu_i}{d}\,d\hat{z}$$

$$\Delta_i(\hat{z}) = \frac{2(-is_+)^{\frac{1}{2}}}{d}\,(\underset{\sim}{T}\cdot\hat{e}_i)\cdot\underset{\sim}{A}_x^{-1}\cdot\vec{g}_t\,\exp\,(k_i^*)$$

where d is the derivative of $c_o^2\eta$ introduced in Eq. (4.8), and where the dependence on ζ and υ has been suppressed. Clearly $\varphi_i(\hat{z})$ and $\Delta_i(\hat{z})$ are analytic for all $0 \le \hat{z} \le \hat{z}_+$ so that we can apply the method of stationary phase[15] to obtain

$$b_{11} = O(\epsilon^{-3/4})$$

$$b_{12} = O(\epsilon^{-3/4}). \qquad (5.10)$$

From the path around the turning point arises the contribution

$$b_{13} = i\delta\int_\pi^0 \vec{\theta}_1\cdot\underset{\sim}{A}_x^{-1}\cdot\vec{g}_t e^{i\varphi}d\varphi\ .$$

Since the integrand is of order $\delta^{-\frac{1}{4}}$ for small δ, it follows that in the limit $\delta \to 0$,

$$b_{13} = 0 \tag{5.11}$$

Finally the contribution beyond the turning point is

$$b_{14} = \int_{x*}^{\infty} \vec{\theta}_1 \cdot \underset{\sim}{A}_x^{-1} \cdot \vec{g}_t dx,$$

and μ_1 is complex with negative real part. A suitable asymptotic bound on b_{14} is obtained for its absolute value,

$$|b_{14}| \leq \int_{x*}^{\infty} e^{-\epsilon\hat{z}(x)} s^{-\frac{1}{2}} \left| s_+^{\frac{1}{2}} (\underset{\sim}{T} \cdot \hat{e}_1) \cdot \underset{\sim}{A}_x^{-1} \cdot \vec{g}_t \exp(k_1^*) \right| dx$$

$$\hat{z} = \int_{x*}^{x} (\kappa s/\eta u) dx'.$$

Now it can be seen that $\hat{z}$ has a power series expansion in s, beginning with the cubic term. Thus conversion to the integration variable $\hat{z}$ yields

$$|b_{14}| \leq \int_0^{\infty} e^{-\epsilon\hat{z}} \hat{z}^{-\frac{1}{2}} \Delta_4(\hat{z}) d\hat{z}$$

$$\Delta_4(\hat{z}) = \left(\frac{\hat{z}}{s^3}\right)^{\frac{1}{2}} \frac{\eta u}{\kappa} \left| s_+^{\frac{1}{2}} (\underset{\sim}{T} \cdot \hat{e}_1) \cdot \underset{\sim}{A}_x^{-1} \cdot \vec{g}_t \exp(k_1^*) \right| .$$

Since $\vec{g}_t$ vanishes exponentially in x and k_i^* has, for $\mathrm{Re}(\upsilon) \geq 0$, negative real part and is linear in x [Eq. (3.8)], it is seen that Δ_4 is bounded, whence

$$|b_{14}| \leq M\int_0^\infty e^{-\epsilon\hat{z}}\hat{z}^{-\frac{1}{2}}d\hat{z} = O(\epsilon^{-\frac{1}{2}}). \tag{5.12}$$

To establish the order of b_1, then, we yet require the order of the coefficient α of b_{12}. But α depends on ϵ only through the integral of μ_1 (i.e., h_1) which is pure imaginary on the $x < x^*$ portion of contour C of Eq. (4.21). Since μ_1 is finite at x^* itself, the portion of C around x^* yields zero in the limit of vanishing radius, whence we obtain

$$\alpha = O(\epsilon^0) \tag{5.13}$$

and we combine Eq. (5.10), (5.11), (5.12), and (5.13) to yield

$$b_1 = O(\epsilon^{-\frac{1}{2}}). \tag{5.14}$$

Identical considerations apply to b_2 as well.

Profiles D and M

The derivation of order relations in both of these cases is similar to that for profile I and in both cases the relation (5.14) is recovered.

Expressions for L

It follows, then, that the b's can be ignored in Eq. (5.1) and only the scalar product remains. For ζ in Class I and Class II, the only contribution to $\vec{\theta}(0, \zeta, \upsilon, \epsilon)$ is that from $\vec{\theta}_1$ which yields

$$L(\epsilon, \zeta, v) \sim L_1(\zeta)$$

$$L_1(\zeta) = -\frac{u_-(1-\nu_v)}{\eta_+}\left[\frac{\ell_+\zeta(\zeta + \kappa_+ s_+)}{u_+u_-} + \eta_+\left(1 - \frac{\zeta^2}{u_+u_-}\right)\right] \tag{5.15}$$

$$\ell = 2 - (1 - \eta)(1 - \nu_v)v_-p_S/T$$

$$\nu_v = v_+/v_- \quad .$$

The new symbols in Eq. (5.15) are T, the temperature, and p_S, the entropy derivative of pressure p at constant volume v and composition $\vec{\lambda}$. Here we have used subscripts + and - to denote evaluation in back of and in front of the shock, respectively. This is simply the value of V for a step shock.[6]

For ζ in Class III, the value of $\vec{\theta}$ at the shock depends upon whether we are considering profile D or profiles I and M. In the former case, we still have $\vec{\theta} \sim \vec{\theta}_1$ so that

$$L \sim L_1(\zeta) \text{ for profile D;} \tag{5.16}$$

but for those cases where $c_o^2\eta$ increases with distance at the shock, we have

$$L \sim L_1(\zeta) + \alpha(\epsilon, \zeta, v)L_2(\zeta), \text{ for profiles I and M} \tag{5.17}$$

where $L_2(\zeta)$ differs from L_1, Eq. (5.15), only in the appearance of $-s_+$ instead of s_+, i.e.,

$$L_2(\zeta) = -\frac{u_-(1-\nu_v)}{\eta_+}\left[\frac{\ell_+\zeta(\zeta - \kappa_+ s_+)}{u_+u_-} + \eta_+\left(1 - \frac{\zeta^2}{u_+u_-}\right)\right] .$$

Determination of α

The coefficient α of the non-shock (L_2) contribution to L for profiles I and M is defined in Eq. (4.21). Letting the radius of the circular part of C approach zero, one finds, using $\underset{\sim}{E}$ from Appendix A, the logarithm of α to be

$$\beta(\epsilon, \zeta, \upsilon) = \ell n\, \alpha(\epsilon, \zeta, \upsilon)$$

$$\beta(\epsilon, \zeta, \upsilon) = \pi i/2 - i\epsilon\beta_1(\zeta_i) + \beta_2(\zeta_i) - \upsilon\beta_3(\zeta_i)$$

$$\beta_1 = \int_0^{x^*(\zeta_i)} \frac{2\kappa|s|\,dx}{\eta u}$$

$$\beta_2 = \zeta_i \int_0^{x^*(\zeta_i)} \frac{\kappa}{\eta|s|}\left[\frac{1}{1-\eta}\frac{d\eta}{dx} - \frac{vp_S}{T}\frac{\vec{\sigma}\cdot\vec{r}}{u}\right. \tag{5.18}$$

$$\left. + \frac{2u\vec{\sigma}\cdot\vec{r}}{(1-\eta)(u^2+\zeta_i^2)} - \frac{v\vec{\sigma}\cdot\vec{r}_v}{u}\right]dx$$

$$\beta_3 = \zeta_i \int_0^{x^*(\zeta_i)} \frac{2\kappa}{\eta|s|u}\,dx$$

$$\zeta = i\zeta_i\ .$$

The subscript v on the rate $\vec{r}$ denotes the partial derivative at constant entropy and composition. We note that β_1, β_2, and β_3 are all real and that β_1 and β_3 are positive but β_2 depends on the equation of state and kinetics of the particular system. For profile I, however, it is seen that β_2 becomes negative for ζ_i^2 sufficiently near the value $(c_o^2\eta)_{x=\infty}$,

and in fact approaches $-\infty$, by virtue of the fact, noted in Sec. 3, that only the $\vec{\sigma} \cdot \vec{r}_v$ term continues to contribute to the integral for large x, and $\vec{\sigma} \cdot \vec{r}_v$ is necessarily positive at chemical equilibrium.

Stability

At the outset, it is expeditious to assume that the equation of state of the unreacted explosive is such that the von Neumann shock is itself stable (i.e., it would be stable if the reactions behind it were somehow suppressed), for we thereby concentrate attention on instability which arises solely from the reactions. Thus, we assume that $L_1(\zeta)$ has no roots in the right half-plane, and in fact we require that its roots have negative real part. It follows that the asymptotic expression for V is non-zero for all Class I and Class II values of ζ, whence <u>any unstable roots</u> are to be found with ζ <u>pure imaginary</u> and in Class III with $\mathrm{Re}(\upsilon) > 0$. Moreover, detonations characterized by profile D are stable for large ϵ, since the shock expression for V holds for Class III values of ζ as well. Thus we now confine our attention to profiles I and M.

Now the behavior of L_1 has been given in the discussion of shock stability,[6] from which it can be seen that our assumption, that $L_1(\zeta)$ only has roots with $\mathrm{Re}(\zeta) < 0$, implies that $L_1(\zeta)$ is positive for $\zeta_i^2 > (c_o^2 \eta)_+$ and increases monotonically with ζ_i (see Case Ib of Ref. 6). Now α, Eq. (4.21) and (5.18), is periodic in ϵ and has magnitude

$$|\alpha| = \exp\left[\beta_2 - \mathrm{Re}(\upsilon)\beta_3\right] .$$

If, therefore, for ζ in Class III, we have the inequality

$$|L_2(i\zeta_i)| \exp [\beta_2(\zeta_i)] < L_1(i\zeta_i), \tag{5.19}$$

it follows that for $\mathrm{Re}(\upsilon) \geq 0$, $L = L_1 + \alpha L_2$ has positive real part irrespective of ϵ and $\mathrm{Im}(\upsilon)$. Hence, for those ζ_i for which Eq. (5.19) holds, V has no unstable roots.

However, if for some ζ_i, we have

$$|L_2(i\zeta_i)| \exp [\beta_2(\zeta_i)] > L_1(i\zeta_i), \tag{5.20}$$

then unstable roots occur for $\mathrm{Re}(\upsilon)$ satisfying

$$L_1 = |L_2| \exp [\beta_2 - \mathrm{Re}(\upsilon)\beta_3] \tag{5.21}$$

at periodically distributed values of $\mathrm{Im}(\upsilon)$, viz.

$$\mathrm{Im}(\upsilon) = [(2n - \tfrac{1}{2})\pi - \epsilon\beta_1]\beta_3^{-1}, \quad L_2 > 0,$$

$$\mathrm{Im}(\upsilon) = [(2n + \tfrac{1}{2})\pi - \epsilon\beta_1]\beta_3^{-1}, \quad L_2 < 0, \tag{5.22}$$

for $n = 0, \pm 1, \ldots$. It follows, then, that every point on the vertical line in the υ-plane satisfying Eq. (5.21) is asymptotically a root of V for periodically distributed values of ϵ,

$$\epsilon = [(2n - \tfrac{1}{2})\pi - \mathrm{Im}(\upsilon)\beta_3]\beta_1^{-1}, \quad L_2 > 0,$$

$$\epsilon = [(2n + \tfrac{1}{2})\pi - \mathrm{Im}(\upsilon)\beta_3]\beta_1^{-1}, \quad L_2 < 0, \tag{5.23}$$

for integer values of n sufficiently large.

To understand the behavior of these roots, we consider the asymptotic expression for V for finite ϵ. Let us suppose that L_1/L_2 and exp (β_2) behave as in Fig. 7, which is appropriate for a $c_o^2\eta$ profile I. The value zero at the right for exp (β_2) occurs by virtue of the approach of β_2 to $-\infty$ as the turning point recedes to $x^* = \infty$. Between ζ_{i1} and ζ_{i2}, Fig. 7, unstable roots occur, as given above, while at ζ_{i1} and ζ_{i2} neutrally stable roots occur. This ζ_i interval is seen to correspond to a series of unstable ϵ-intervals, which for $\mathrm{Im}(\upsilon) = 0$ are

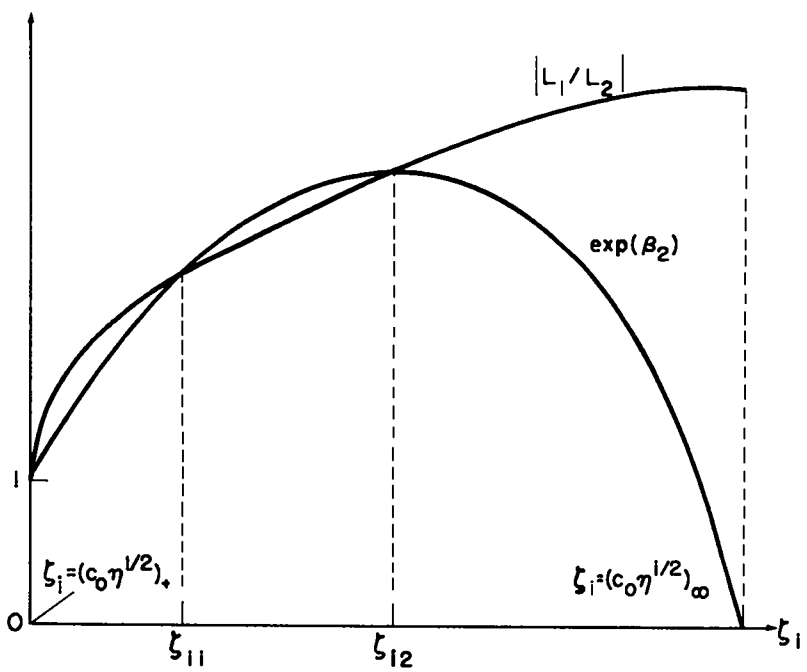

Fig. 7 Sketch of the functions $|L_1/L_2|$ and exp (β_2) for profile I (see Fig. 5) detonations for $\zeta_i = \mathrm{Im}(\tau)/\epsilon$ traversing the Class III segment of the ζ-plane. Instability is obtained in the $\epsilon \to \infty$ limit for a detonation which has exp (β_2) greater than $|L_1/L_2|$, as in the interval (ζ_{i1}, ζ_{i2}).

$$(2n - \tfrac{1}{2})\pi/\beta_1(\zeta_{i2}) < \epsilon < (2n - \tfrac{1}{2})\pi/\beta_1(\zeta_{i1}), \tag{5.24}$$

for n = 1, 2, ... As n increases these intervals overlap, so that for ϵ above some value all wave numbers are unstable and no estimate of the range of unstable ϵ values is obtained. If the exp (β_2) and L_1/L_2 curves do not cross, then no unstable roots occur for large ϵ.

Two additional points should be noted. First we observe that L_1 and L_2 are equal at $\zeta_i^2 = (c_o^2\eta)_+$. Since we had $\alpha = 0$ at $\zeta_i^2 = (c_o^2\eta)_{x=\infty}$ for profile I, it follows that the asymptotic expression for V behaves continuously as ζ_i traverses the boundaries between Class I and Class III for profile I as well as profile D. Because of this continuity, the asymptotic value of V for $\zeta_i^2 = (c_o^2\eta)_{x=\infty}$, a point excluded from all our considerations, is taken simply $V = \epsilon L_1(\zeta)$, as is obtained by approach to this point from either Class I or Class III.

A second point for considerations is concerned with profile M. It is evident that V behaves continuously with ζ_i both at $\zeta_i^2 = (c_o^2\eta)_+$ and $\zeta_i^2 = (c_o^2\eta)_{x=\infty}$. At the maximum value of $c_o^2\eta$, however, continuous behavior can be lacking. Although β_2 does become infinite at this point, as can be seen from Eq. (5.18), its sign can be either + or - simply on the basis of the kinetic coefficients $\vec{r}_v$. If $\beta_2 \to +\infty$, α is also infinite, whence L_2 dominates L_1, while for $\zeta_i^2 > (c_o^2\eta)_{max}$, only the L_1 term appears in the asymptotic formula. It is clear, then, that the complete stability behavior of profile M requires an asymptotic expansion for $\vec{\theta}$, valid at the maximum. This task is reserved for the next section.

6. TURNING-POINT PROBLEM FOR AN EXTREMUM IN $c_o^2\eta$

Although the method of Sec. 4 can presumably be employed to solve the continuation problem facing us here, it is certainly a far more difficult problem. In particular, the discussion of Ref. 5 indicates the need to solve a connection problem of a rather difficult sort. Instead, we turn to the so-called "related-equation method" of Langer, with the hope that much of the present problem has already been solved in its essentials by virtue of the known solution of certain turning-point problems for second-order equations. These second-order equations, of the form

$$\frac{d^2u}{dx^2} + \left[\hat{\omega}^2 q_0(x) + \hat{\omega} q_1(x) + R(x, \hat{\omega})\right] u = 0$$

$$R = \sum_{i=0}^{\infty} r_i(x)/\hat{\omega}^i \tag{6.1}$$

(the absence of a term in du/dx implies no loss of generality[9]), have been solved asymptotically in $\hat{\omega}$ for the case of a simple zero[9] of $q_0(x)$ and a second-order zero.[10] By writing Eq. (6.1) as a system

$$\begin{aligned} u_1 &= u \\ \frac{du_1}{dx} &= \hat{\omega} u_2 \\ d\vec{u}/dx &= \hat{\omega} \underset{\sim}{Q} \cdot \vec{u} \\ \underset{\sim}{Q} &= \begin{bmatrix} 0 & 1 \\ -(q_0 + q_1/\hat{\omega} + R/\hat{\omega}^2 & 0 \end{bmatrix} \end{aligned} \tag{6.2}$$

we see that the simple zero corresponds to the problem of Sec. 4 in so far as the difference in the eigenvalues of the leading matrix vanishes as $(x - x^*)^{\frac{1}{2}}$, while the case of a second-order zero of $q_0(x)$ coincides, in the same sense with the problem at hand. The present section is based upon the exploration of this correspondence.

The procedure which will be followed is as follows. Non-singular transformations of our equations are devised which yield a second-order system of the form of Eq. (6.2) and an (n + 2)-order system, with interactions between the two systems first appearing with terms of order ϵ^{-m} in the coefficient matrix, for arbitrary m. The related equations are taken to be independent systems of order 2 and order n + 2, with coefficient matrices agreeing with the transformed system also to order ϵ^{-m}. The significance of the related equations derives from the fact that their solutions are known. In particular, the related equation of order 2 is taken to be the related equation of McKelvey,[10] while the asymptotic series given by Friedrichs form the related-equation solutions for the (n + 2)-order equations. The proof that there are actual solutions asymptotic to the related-equation solutions has essentially been given by McKelvey and is not detailed here.

Related Equation

We begin once more with Eq. (2.7b)

$$\frac{d\vec{\theta}}{dx} = [\epsilon \underset{\sim}{\Phi}_0(x) + \underset{\sim}{\Phi}_1(x)] \cdot \vec{\theta} \tag{6.3}$$

and restrict our attention henceforth to Class III values of ζ and suppose that the x interval under consideration contains a single turning point. We wish to obtain a related equation, for any integer $m \geq 1$,

$$\frac{d\vec{\varphi}}{dx} = \left[\epsilon \underset{\sim}{\Phi}_0(x) + \underset{\sim}{\Phi}_1(x) + \epsilon^{-m} \underset{\sim}{R}(x, \epsilon) \right] \cdot \vec{\varphi}$$

$$\underset{\sim}{R}(x, \epsilon) = \sum_{\nu=0}^{\infty} \epsilon^{-\nu} \underset{\sim}{R}_\nu(x) \tag{6.4}$$

such that a complete system of $n + 4$ solutions of Eq. (6.4) are known.

To accomplish this task, we proceed inversely by transforming Eq. (6.3) so that it will resemble equations with known solutions. We look for a similarity transform

$$\vec{\theta} = \underset{\sim}{S}_0(x, \epsilon) \cdot \vec{\Psi}_{(0)}$$

$$\underset{\sim}{S}_0 = \underset{\sim}{Q}_0(x) \exp \left[\tfrac{1}{2} \epsilon \int_0^x (\mu_1 + \mu_2) dx' \right] \tag{6.5}$$

such that, to highest order in the coefficient matrix, the $\vec{\Psi}_{(0)}$ differential equation will be composed of a second-order equation of the form Eq. (6.2) and a diagonal, $(n + 2)$-order system. In the $\vec{\Psi}_{(0)}$ equations,

$$\frac{d\vec{\psi}(0)}{dx} = \left[\epsilon \underset{\sim}{L}_0(x) + \underset{\sim}{H}(x)\right] \cdot \vec{\psi}(0)$$

$$\underset{\sim}{L}_0(x) = \underset{\sim}{Q}_0^{-1} \cdot \left[\underset{\sim}{\Phi}_0 - \tfrac{1}{2}(\mu_1 + \mu_2)\underset{\sim}{I}\right] \cdot \underset{\sim}{Q}_0 \tag{6.6}$$

$$\underset{\sim}{H}(x) = \underset{\sim}{Q}_0^{-1} \cdot \left[\underset{\sim}{\Phi}_1 \cdot \underset{\sim}{Q}_0 - d\underset{\sim}{Q}_0/dx\right]$$

(the dependence on ζ and υ being suppressed for the present) we observe that $\underset{\sim}{L}_0$ has, in view of Eq. (3.5), eigenvalues, $\frac{1}{2}\mu_{12}$, $\frac{1}{2}\mu_{21}$, and $\mu_{31} - \frac{1}{2}\mu_{21}$ whence we require $\underset{\sim}{L}_0$ be given by

$$\underset{\sim}{L}_0 = \begin{bmatrix} 0 & 1 & 0 \\ -\ell_0(x) & 0 & \\ 0 & & n(x)\underset{\sim}{I}_{n+2} \end{bmatrix} \tag{6.7}$$

$$\ell_0(x) = -\mu_{21}^2/4 = -(1-\eta)(\zeta^2 + c_o^2\eta)/\eta^2 u^2$$

$$n(x) = \mu_{31} - \mu_{21}/2 = \zeta/\eta u$$

where $\underset{\sim}{I}_i$ denotes the unit matrix of order i. It is important to note that the exponential in Eq. (6.5) and the matrix $\underset{\sim}{L}_0$ do not contain algebraic branch points at a turning point, for the square root s does not appear. Thus, $\underset{\sim}{Q}_0(x)$ can be found as a regular function of x, and this determination is given in Appendix C. In addition $\underset{\sim}{Q}_0$ is a non-singular matrix (i.e., $|\underset{\sim}{Q}_0| \neq 0$) for all x. In view of these properties of $\underset{\sim}{Q}_0$, it is clear that $\underset{\sim}{H}(x)$, Eq. (6.6), is a regular function of x.

To proceed further, we look for additional similarity transforms which will turn the lower-order matrices of the differential equation into block-diagonal form, with the upper 2-by-2 of the special form displayed by Eq. (6.2), and at the same time not affect the leading matrices which are already in this form. The existence of such matrices, of the form

$$\underset{\sim}{S}_k = [\underset{\sim}{I} + \epsilon^{-k}\underset{\sim}{Q}_k(x)] \quad \exp\left[\epsilon^{-k+1}\int_0^x g_{k-1}(x')dx'\right], \tag{6.8}$$

for $k \geq 1$, is suggested by the work of Turrittin.[16] We let

$$\vec{\theta} = \underset{\sim}{S}^{(k)} \cdot \vec{\psi}_{(k)}$$

$$\underset{\sim}{S}^{(k)} = \underset{\sim}{S}_0 \cdot \underset{\sim}{S}_1 \cdots \underset{\sim}{S}_k \tag{6.9}$$

and require that

$$\frac{d\vec{\psi}_{(k)}}{dx} = \epsilon\underset{\sim}{\Lambda}_k(x, \epsilon) \cdot \vec{\psi}_{(k)}$$

$$\underset{\sim}{\Lambda}_k(x, \epsilon) = \underset{\sim}{L}^{(k)}(x, \epsilon) + \epsilon^{-(k+1)}\underset{\sim}{U}^{(k)}$$

$$\underset{\sim}{L}^{(k)}(x, \epsilon) = \sum_{\nu=0}^{k} \epsilon^{-\nu}\underset{\sim}{L}_\nu(x) \tag{6.10}$$

$$\underset{\sim}{U}^{(k)}(x, \epsilon) = \sum_{\nu=0}^{\infty} \underset{\sim}{U}_\nu^{(k)}(x)\epsilon^{-\nu}$$

$$\underset{\sim}{L}_\nu(x) = \begin{bmatrix} 0 & 0 & \\ -\ell_\nu(x) & 0 & 0 \\ & & \\ 0 & & \underset{\sim}{N}_\nu(x) \end{bmatrix}, \quad \nu \geq 1 \quad .$$

The proof that such $\underset{\sim}{S}_k$ exists is also given in Appendix C and, again, these transforms are regular functions of x. Obviously each $\underset{\sim}{S}_k$ has an inverse for ϵ sufficiently large.

For any given integer m, the transformations in Eq. (6.9) can be terminated to yield

$$\begin{aligned}
&\vec{\Psi}(x, \epsilon) = \vec{\Psi}_{(m)}(x, \epsilon) \\
&\underset{\sim}{U}(x, \epsilon) = \underset{\sim}{U}^{(m)}(x, \epsilon) = \sum_{\nu=0}^{\infty} \epsilon^{-\nu} \underset{\sim}{U}_\nu(x) \\
&\underset{\sim}{L}(x, \epsilon) = \underset{\sim}{L}^{(m)}(x, \epsilon) \\
&\underset{\sim}{S}(x, \epsilon) = \underset{\sim}{S}^{(m)}(x, \epsilon) \\
&\frac{d\vec{\Psi}}{dx} = [\epsilon \underset{\sim}{L}(x, \epsilon) + \epsilon^{-m} \underset{\sim}{U}(x, \epsilon)] \cdot \vec{\Psi} \quad .
\end{aligned} \tag{6.11}$$

If solutions $\vec{y}(x, \epsilon)$ of an equation resembling Eq. (6.11)

$$\begin{aligned}
&\frac{d\vec{y}}{dx} = [\epsilon \underset{\sim}{L} + \epsilon^{-m} \underset{\sim}{J}(x, \epsilon)] \cdot \vec{y} \\
&\underset{\sim}{J}(x, \epsilon) = \sum_{\nu=0}^{\infty} \epsilon^{-\nu} \underset{\sim}{J}_\nu(x)
\end{aligned} \tag{6.12}$$

are known, we will refer to Eq. (6.12) as the transformed related equation, for it is readily seen that

$$\vec{\varphi} = \underset{\sim}{S}_0 \cdot \underset{\sim}{S}_1 \cdots \underset{\sim}{S}_m \cdot \vec{y} = \underset{\sim}{S} \cdot \vec{y} \tag{6.13}$$

satisfies an equation of the form of Eq. (6.4). In fact, we find

$$\underset{\sim}{R}(x, \epsilon) = \underset{\sim}{S} \cdot (\underset{\sim}{J} - \underset{\sim}{U}) \cdot \underset{\sim}{S}^{-1} \tag{6.14}$$

which has the desired power series expansion, since the exponential factors in the $\underset{\sim}{S}_\nu$ cancel in Eq. (6.14) while the $(\underset{\sim}{I} + \epsilon^{-\nu}\underset{\sim}{Q}_\nu)^{-1}$ matrices have well-known power series expansions for ϵ sufficiently large. Thus, we regard both Eq. (6.4) and Eq. (6.12) as related equations.

Solution of the Related Equation

Now it is clear that the matrix $\underset{\sim}{J}$ in Eq. (6.12) is to be chosen to have the special black-diagonal form of the $\underset{\sim}{L}_\nu (\nu \geq 1)$ matrices; for then Eq. (6.12) decomposes into two <u>independent</u> differential equations

$$\frac{d^2y}{dx^2} + [\epsilon^2 \ell_0 + \epsilon \ell_1 + q(x, \epsilon)]\, y = 0$$

$$y(x, \epsilon) = \vec{y}(x, \epsilon) \cdot \hat{e}_1$$

$$q(x, \epsilon) = \sum_{\nu=0}^{m-2} \epsilon^{-\nu} \ell_{\nu+2}(x) + \epsilon^{-m+1} e(x, \epsilon) \qquad (6.15)$$

$$\frac{d\vec{\rho}}{dx} = [\epsilon \underset{\sim}{N}(x, \epsilon) + \epsilon^{-m} \underset{\sim}{M}(x, \epsilon)] \cdot \vec{\rho}$$

$$\underset{\sim}{N}(x, \epsilon) = \sum_{\nu=0}^{m} \epsilon^{-\nu} \underset{\sim}{N}_\nu(x)\,, \qquad (6.16)$$

where $\vec{\rho}$ is the projection of $\vec{y}$ onto the lower $(n + 2)$-space and where we have written

$$\underset{\sim}{J}(x, \epsilon) = \begin{bmatrix} 0 & 0 & \\ & & 0 \\ -e(x, \epsilon) & 0 & \\ & & \\ 0 & & \underset{\sim}{M}(x, \epsilon) \end{bmatrix} .$$

Equation (6.15) is the type discussed by Langer and McKelvey and we will choose $e(x, \epsilon)$ so that it is precisely their related equation. We can first dispose of the $\vec{\rho}$ equation, irrespective of the nature of the turning point, i.e., irrespective of the order of the zero of ℓ_0, Eq. (6.7).

Solution of the (n + 2)-order system

Now Eq. (6.16) is of the type considered in Sec. 3 and 4 except that there are no turning points; instead the eigenvalues of the leading matrix, $n(x)$, are everywhere identical, and series solutions can be derived by the method described by Friedrichs.[5] Thus, we set

$$\vec{\rho}(x, \epsilon) = \vec{c}(x, \epsilon) \exp\left[\epsilon \int_0^x n(x')dx'\right] \qquad (6.17)$$

whence

$$\frac{d\vec{c}}{dx} = \left[\underset{\sim}{N}_1(x) + \frac{1}{\epsilon}\underset{\sim}{N}_2(x) + \cdots + \frac{1}{\epsilon^{m-1}}\underset{\sim}{N}_m + \frac{1}{\epsilon^m}\underset{\sim}{M}\right] \cdot \vec{c} . \qquad (6.18)$$

We now demonstrate that, for proper choice of $\underset{\sim}{M}$, Eq. (6.18) has a complete set of n + 2 independent solutions which are polynomials in $1/\epsilon$,

$$\vec{c} = \sum_{\nu=0}^{p} \epsilon^{-\nu}\vec{c}_\nu , \qquad (6.19)$$

with the degree p as yet unspecified. Substitution into Eq. (6.18) yields

$$\sum_{\nu=0}^{p}\epsilon^{-\nu}\vec{dc}_\nu/dx = \sum_{\nu=0}^{p}\sum_{\mu=0}^{m-1}\epsilon^{-\mu-\nu}\underset{\sim}{N}_{\mu+1}\cdot\vec{c}_\nu + \epsilon^{-m}\underset{\sim}{M}\cdot\vec{c}\ . \tag{6.20}$$

Equating coefficients of $\epsilon^{-\nu}$ for $\nu < m$, we obtain relations independent of $\underset{\sim}{M}$,

$$\frac{\vec{dc}_\nu}{dx} = \underset{\sim}{N}_1\cdot\vec{c}_\nu + \sum_{\mu=1}^{\nu}\underset{\sim}{N}_{\mu+1}\cdot\vec{c}_{\nu-\mu},\ \nu < m \tag{6.21}$$

in which we define $\vec{c}_k = 0$, for $k > p$, the degree of the polynomial. The first of these relations (for $\nu = 0$) is seen to be a linear homogeneous differential equation and has n + 2 independent solutions which form the columns of the solution matrix $\underset{\sim}{C}_0(x)$, which can be specified uniquely by the initial data,

$$\underset{\sim}{C}_0(0) = \underset{\sim}{I}_{n+2}\ . \tag{6.22}$$

The remainder of the differential equations (6.21), i.e., $\nu \le \min(m - 1, p)$, are inhomogeneous, with inhomogeneous terms dependent only on $\vec{c}_k$ with $k < \nu$. Therefore, these can be solved serially in terms of the solution matrix $\underset{\sim}{C}_0$ of the homogeneous part. In particular, we obtain a set of n + 2 solutions for each ν, namely

$$\underset{\sim}{C}_\nu = \underset{\sim}{C}_0(x)\cdot\int_0^x \underset{\sim}{C}_0^{-1}(s)\cdot\sum_{\mu=1}^{\nu}\underset{\sim}{N}_{\mu+1}(s)\cdot\underset{\sim}{C}_{\nu-\mu}(s)ds. \tag{6.23}$$

Now it can be seen that the degree p of the polynomial $\vec{c}$ cannot be less than m - 1, for Eq. (6.21) would yield for $p < \nu \le m - 1$ an

algebraic linear relation among the $\vec{c}_k$, $k < \nu$, which is not in general satisfied. Hence, we have $p \geq m - 1$, and in fact it suffices to choose $p = m - 1$.

Now if we remove the early powers in $1/\epsilon$ from Eq. (6.20) through Eq. (6.21) and let $\underset{\sim}{C}$ denote the matrix of polynomials $\vec{c}$, viz.,

$$\underset{\sim}{C} = \sum_{\nu=0}^{m-1} \epsilon^{-\nu} \underset{\sim}{C}_\nu \ , \tag{6.24}$$

then Eq. (6.20) is found to determine $\underset{\sim}{M}$,

$$\underset{\sim}{M} = - \sum_{\nu=1}^{m-1} \epsilon^{-\nu+1} \sum_{\mu=\nu}^{m-1} \underset{\sim}{N}_{\mu+1} \cdot \underset{\sim}{C}_{m+\nu-1-\mu} \cdot \underset{\sim}{C}^{-1} \ . \tag{6.25}$$

Since $\underset{\sim}{C}^{-1}$ has a power series expansion for ϵ sufficiently large, it follows that the $\underset{\sim}{M}$ contribution to $\underset{\sim}{J}(x, \epsilon)$ has the power series expansion required by Eq. (6.12). A complete set of solutions for Eq. (6.18) are, therefore, known, and through Eq. (6.17) the solutions $\vec{\rho}$ of Eq. (6.16) are given.

Solution of the second-order equation

To find solutions for Eq. (6.15), we must now specialize to a particular turning-point problem. Without appreciable increase in effort, we can simultaneously treat both types of extrema in $c_o^2 \eta$. In order to apply the formulas of McKelvey[10] for the so-called second-order

turning-point problem, we transform thus:†

$$\hat{\omega} = \delta\epsilon$$

$$\delta = i \qquad \text{for } d^2\ell_0/dx^2 > 0 \text{ at } x^*$$

$$\delta = 1 \qquad \text{for } d^2\ell_0/dx^2 < 0 \text{ at } x^*$$

$$z = x - x^*$$

$$u(z, \hat{\omega}) = y(x^* + z, \hat{\omega}/\delta) \tag{6.26}$$

$$p_0(z) = -\delta^{-2}\ell_0(x^* + z)$$

$$p_1(z) = -\delta^{-1}\ell_1(x^* + z)$$

$$Q(z, \hat{\omega}) = -q(x^* + z, \hat{\omega}/\delta) = \sum_{j=0}^{\infty} q_j(z)\hat{\omega}^{-j}$$

to provide a notation similar to Ref. 10. The final equation defines the low-order terms q_j in terms of the low-order terms of Eq. (6.15). The latter equation becomes

$$\frac{d^2u}{dz^2} - [\hat{\omega}^2 p_0(z) + \hat{\omega}p_1(z) + Q(z, \hat{\omega})]\, u = 0, \tag{6.27}$$

and Eq. (6.27) satisfies the hypotheses made by McKelvey. In particular, note that $p_0(z)$ is non-negative for real values of z. [It should be

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† The reader is cautioned that several specialized symbols are introduced and used, particularly between this point and the end of this subsection. Many resemble symbols used elsewhere in the report, but differ in some detail. Thus, in Eq. (6.26), u, p_0, and p_1 are not to be confused with mass velocity and pressure. In addition, the independent variable z differs from that of Sec. 4 and 5 by virtue of a translation of the origin by x^*, but the symbol is identical.

recalled that we restricted attention to an interval containing only a single zero of $\ell_0(x)$.] Following McKelvey, we define

$$\phi(z, \hat{\omega}) = p_0(z)^{\frac{1}{2}}$$

$$\psi(z, \hat{\omega}) = 2\hat{\omega}\int_0^z \phi(z)dz \tag{6.28}$$

$$\Pi(z) = \frac{\left[\int_0^z \phi(z)dz\right]^{\frac{1}{4}}}{\phi(z)^{\frac{1}{2}}} .$$

Note that $\phi(z)$ is analytic for all real z if we let arg $\phi = 0$ for $z > 0$ and arg $\phi = \pi$ for $z < 0$. Thus, arg ψ = arg $\hat{\omega}$ for $z > 0$ and arg $\psi = 2\pi$ + arg $\hat{\omega}$ for $z < 0$. [For arg$(\hat{\omega})$, we use, of course, either 0 or $\pi/2$.] Finally we note that Π is regular and non-zero at $z = 0$. The introduction of the variable ψ has the character of a "stretching transformation" since it appears in the final solution below as the independent variable in the differential equation for the leading part of the solution.

Now McKelvey has shown that the behavior of the solutions of Eq. (6.27) for large $|\hat{\omega}|$ depends essentially only on $p_0(z)$ and $p_1(z)$ and that the solutions are asymptotically given by the confluent hypergeometric functions, [17] both for finite z and for the neighborhood of $z = 0$. In particular, for proper choice of the function $e(x, \epsilon)$, Eq. (6.15), McKelvey has shown that Eq. (6.27) has series solutions of the form,

$$u_\nu(z, \hat{\omega}) = \Upsilon(z, \hat{\omega})^{-\frac{1}{2}}[A(z, \hat{\omega})v_\nu(z, \hat{\omega}) + B(z, \hat{\omega})v_\nu'(z, \hat{\omega})/\hat{\omega}] \tag{6.29a}$$

where the prime denotes the derivative with respect to the spatial coordinate and where subscript ν appears explicitly, not only to label the independent solutions but also to show that the polynomials A and B,

$$A(z, \hat{\omega}) = \sum_{i=0}^{m-2} a_i(z)\hat{\omega}^{-1}$$

$$B(z, \hat{\omega}) = \sum_{i=0}^{m-2} b_i(z)\hat{\omega}^{-1}, \tag{6.29b}$$

are independent of ν. The leading term in these solutions will be our principal interest, so we observe[10] that

$$a_0(z) = \cosh j(z)$$

$$b_0(z) = \phi^{-1} \sinh j(z) \tag{6.29c}$$

$$j(z) = \int_0^z \frac{p_1(z') - p_1(0)\Pi^4(0)/\Pi^4(z')}{2\phi(z')} dz' .$$

It is important to note that $j(z)$ is regular at the turning point, $z = 0$. We have for Υ the determinant

$$\Upsilon(z, \hat{\omega}) = \begin{vmatrix} A & B/\hat{\omega} \\ A' + B\Sigma/\hat{\omega} & A + B'/\hat{\omega} \end{vmatrix}$$

$$\Sigma = \hat{\omega}^2 p_0(z) + \hat{\omega} p_1(0)\Pi^4(0)/\Pi^4(z) + \Pi''(z)/\Pi(z) + k(\hat{\omega}) \tag{6.29d}$$

$$k(\hat{\omega}) = \sum_{i=0}^{m-2} k_i \hat{\omega}^{-i}$$

$$k_0 = -\tfrac{1}{2} p_1(0)\Pi^4(0) .$$

Finally, the functions $v_\nu(z, \hat{\omega})$ are essentially the solutions of the leading part of the differential equation and are conveniently written

$$v_\nu(z, \hat{\omega}) = \Pi(z)\psi^{-\frac{1}{4}}W_\nu[\psi, k(\hat{\omega})] \quad . \tag{6.29e}$$

The W_ν, which are of central importance in the sequel, are independent solutions of the confluent hypergeometric equation[17]

$$\frac{d^2W_\nu}{d\psi^2} + \left[-\tfrac{1}{4} + \frac{k}{\psi} + \frac{\frac{1}{4} - p^2}{\psi^2} \right] W_\nu = 0, \tag{6.30}$$

for the special value $p = \frac{1}{4}$.

Now the choice of the function $e(x, \epsilon)$ whereby the $u_\nu(z, \hat{\omega})$ become the exact solutions of the second-order related equation need not concern us (beyond the fact of its existence). Instead we now concentrate attention on describing the behavior of these u_ν functions along the (real) z axis, particularly with regard to the analytic continuation through the turning point at $z = 0$.

Now the neighborhood of $z = 0$ is seen from Eq. (6.28) to correspond to finite values of ψ for which the u_ν functions can be found through the power series expansions of the confluent hypergeometric functions,[18]

$$W_\nu(\psi, k) = M_{k,p}(\psi)$$

$$M_{k,p}(\psi) = \psi^{\frac{1}{2}+p}e^{-\frac{1}{2}\psi}\left[1 + \frac{\frac{1}{2} + p - k}{2p + 1}\psi + \ldots\right] \tag{6.31}$$

$$p = \tfrac{1}{4}, -\tfrac{1}{4}.$$

Although of considerable importance in proving that the given differential equation and the related equation are equivalent asymptotically, these relations are of no practical importance in obtaining the desired asymptotic estimates for the u_ν functions. With regard to the latter point, we need to consider only non-zero values of z for which the asymptotic behavior of the W_ν is seen to be important. Thus, for large $|\hat{\omega}|$, we evaluate Eq. (6.29a), using for Υ the result from Eq. (6.29c) and (6.29d)

$$\Upsilon \sim 1,$$

whence we obtain

$$u_\nu(z, \hat{\omega}) \sim \Pi(z)\ \psi^{-\frac{1}{4}} \left[\cosh\ j(z) W_\nu(\psi, k_0) + 2\ \sinh\ j(z)\ \frac{dW_\nu(\psi, k_0)}{d\psi}\right] . \tag{6.32}$$

Moreover, the derivative of u_ν, which enters into the vector solutions $\vec{y}$, Eq. (6.12), is found, on using the differential Eq. (6.30) to evaluate the second derivative of W_ν, to satisfy for non-zero z

$$\frac{du_\nu}{dz} \sim \hat{\omega}\phi\Pi\psi^{-\frac{1}{4}} \left[2\ \cosh\ j(z)\ \frac{dW_\nu(\psi, k_0)}{d\psi} + \sinh\ j(z) W_\nu(\psi, k_0)\right] . \tag{6.33}$$

Now rather than use the $M_{k,p}$ hypergeometric functions, Eq. (6.31), it is more convenient for purposes of asymptotic analysis to use the Whittaker functions which can be defined[19] as

$$W_{k,p}(\psi) = \frac{\Gamma(-2p)}{\Gamma(\frac{1}{2}-p-k)} M_{k,p}(\psi) + \frac{\Gamma(2p)}{\Gamma(\frac{1}{2}+p-k)} M_{k,-p}(\psi) \tag{6.34}$$

and particularly the variant given by McKelvey[10]

$$W_{\nu}(\psi) = W_{\sigma k,\frac{1}{4}}(\psi e^{-\nu\pi i}), \quad \nu = 0, \pm 1, \pm 2, \ldots$$

$$\sigma = (-1)^{\nu} \tag{6.35}$$

in which the argument of the product of complex numbers is understood to be the sum of their arguments, and where

$$\arg(e^{-\nu\pi i}) = -\nu\pi .$$

These have the asymptotic form,[20]

$$W_{\nu}(\psi) = e^{-\frac{1}{2}\sigma\psi} (\psi e^{-\nu\pi i})^{\sigma k}[1 + O(1/\psi)], \text{ for } \psi \text{ on } \Sigma_{\nu}$$

$$\Sigma_{\nu}: (\nu - 3/2)\pi < \arg \psi < (\nu + 3/2)\pi . \tag{6.36}$$

The asymptotic behavior of the derivative of W_{ν} follows from the derivative of the Whittaker functions[21]

$$\frac{dW_{k,p}}{d\psi} = \psi^{-1}\left\{ (k - \tfrac{1}{2}\psi)W_{k,p} - [p^2 - (k - \tfrac{1}{2})^2]W_{k-1,p}\right\}$$

whence

$$\frac{dW_{\nu}}{d\psi} \sim -\tfrac{1}{2}e^{-\nu\pi i}W_{\nu}, \quad \text{for } \psi \text{ on } \Sigma_{\nu} . \tag{6.37}$$

Now it is evident from the definition of the Σ_ν intervals that Eq. (6.36) and (6.37) are not sufficient to complete the expansions of u_ν, Eq. (6.32) and (6.33), for z both positive and negative. Therefore we require a continuation formula for the W_ν functions. For this purpose, we employ Kummer's "first" formula[22] which is particularly convenient in the form given by McKelvey[10]

$$M_{k,p}(\psi) = i^{\nu} e^{p\nu\pi i} M_{\sigma k,p}(\psi e^{-\nu\pi i})$$

for ν any signed integer or zero. Using this result in conjunction with the definitions, Eq. (6.34) and (6.35), and employing the "reflection" formula[23] for the gamma functions, we obtain

$$W_\nu(\psi) = \frac{2\pi i e^{\sigma k\pi i}}{\Gamma(\frac{1}{4}-\sigma k)\Gamma(3/4-\sigma k)} W_{\nu+1}(\psi) + e^{2\sigma k\pi i} W_{\nu+2}(\psi) \qquad (6.38a)$$

connecting three "adjacent" W_ν functions and

$$W_\nu(\psi) = -e^{-2\sigma k\pi i} W_{\nu+2}(\psi) + \frac{2\pi i e^{-\sigma k\pi i}}{\Gamma(\frac{1}{4}-\sigma k)\Gamma(3/4-\sigma k)} W_{\nu+3}(\psi) \, . \qquad (6.38b)$$

It is evident that Eq. (6.38a) permits the continuation of the asymptotic expression for W_ν from Σ_ν to the intersection $\cap(\Sigma_{\nu+1}, \Sigma_{\nu+2})$ while Eq. (6.38b) permits extension to $\cap(\Sigma_{\nu+2}, \Sigma_{\nu+3})$. These sectors are found to overlap, and further continuation is given by application of the formula,

$$W_\nu(\psi) = - W_{\nu+4}(\psi), \qquad (6.38c)$$

which is obtained in the same manner indicated above.

Now it can be shown that any pair of four "adjacent" W_ν are linearly independent [except for special positive values of $k = \frac{1}{4}$ or $3/4$ (mod 1), for which only adjacent pairs are independent]. It is convenient, for the purpose of finally solving the stability problem, to consider the $\nu = 0$ and $\nu = 2$ pair and to obtain from these u_ν functions the corresponding solutions of the original second-order related equation, Eq. (6.12),

$$\vec{y}^{(\nu)}(x, \epsilon) = \begin{bmatrix} u_\nu(z, \hat{\omega}) \\ \epsilon^{-1} du_\nu/dz \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{6.39}$$

We compute now asymptotic expressions for $\vec{y}^{(0)}$ on $z > 0$, where $\arg(\psi) = 0$ or $\pi/2$, by using Eq. (6.36) and (6.37) directly in Eq. (6.32) and (6.33) to obtain

$$\vec{y}^{(0)}(x, \epsilon) \sim \begin{bmatrix} 1 \\ -\kappa s/\eta u \\ 0 \\ 0 \\ 0 \end{bmatrix} \Pi(z) e^{-(\frac{1}{2}\psi + j)} \psi^{k-\frac{1}{4}}, \quad z > 0 \tag{6.40a}$$

where Φ has been evaluated explicitly from Eq. (6.7), (6.26) and (6.28). For $z < 0$, $\arg \psi = 2\pi$ or $5\pi/2$, so that we employ the continuation formula (6.38b) for W_0 and thence expand W_2, W_3 and their derivatives to obtain

$$\vec{y}^{(0)}(x,\epsilon) \sim \begin{bmatrix} 1 \\ -\kappa s/\eta u \\ 0 \\ 0 \\ 0 \end{bmatrix} \frac{2\pi i e^{2k\pi i}}{\Gamma(\frac{1}{4}-k)\Gamma(3/4-k)} \Pi(z) e^{\frac{1}{2}\psi + j\psi - k - \frac{1}{4}}$$

$$- \begin{bmatrix} 1 \\ \kappa s/\eta u \\ 0 \\ 0 \\ 0 \end{bmatrix} \Pi(z) e^{-(\frac{1}{2}\psi + j)\psi^{k-\frac{1}{4}} e^{-4k\pi i}}, \quad z < 0. \tag{6.40b}$$

In similar fashion, we obtain

$$\vec{y}^{(2)}(x,\epsilon) \sim \begin{bmatrix} 1 \\ \kappa s/\eta u \\ 0 \\ 0 \\ 0 \end{bmatrix} \frac{-2\pi i}{\Gamma(\frac{1}{4}-k)\Gamma(3/4-k)} \Pi(z) e^{\frac{1}{2}\psi + j\psi - k - \frac{1}{4}} \tag{6.41a}$$

$$+ \begin{bmatrix} 1 \\ -\kappa s/\eta u \\ 0 \\ 0 \\ 0 \end{bmatrix} \Pi(z) e^{-(\frac{1}{2}\psi + j)\psi^{k-\frac{1}{4}} e^{-2k\pi i}}, \quad z > 0$$

$$\vec{y}^{(2)}(x,\epsilon) \sim \begin{bmatrix} 1 \\ \kappa s/\eta u \\ 0 \\ 0 \\ 0 \end{bmatrix} \Pi(z) e^{-(\frac{1}{2}\psi + j)\psi^{k-\frac{1}{4}} e^{-2k\pi i}}, \quad z < 0. \tag{6.41b}$$

We could, in similar manner, determine additional solutions $\vec{y}^{(1)}$ and $\vec{y}^{(3)}$ but shall not do so here, for we have no need for these in obtaining the asymptotic formula for $\vec{\theta}$.

We have now obtained a total of n + 4 solutions of the related Eq. (6.12), and we denote these $\vec{y}_1, \vec{y}_2, \cdots, \vec{y}_{n+4}$, where

$$\vec{y}_1(x, \epsilon) = \vec{y}^{(0)}(x, \epsilon)$$

$$\vec{y}_2(x, \epsilon) = \vec{y}^{(2)}(x, \epsilon), \tag{6.42}$$

while the remainder are formed from the n + 2 solutions $\vec{\rho}(x, \epsilon)$ given in Eq. (6.17), (6.19), and (6.23). The final problem is to prove that there exist solutions $\vec{\psi}$ of the given Eq. (6.11) which agree with these $\vec{y}_\nu$ up to terms of order ϵ^{-m}, where m is the arbitrary positive integer selected in advance. The method of proof follows closely that of Langer[9] and is sketched in Appendix D. Based on this proof, we have

$$\vec{\psi}_\nu(x, \epsilon) = \vec{y}_\nu(x, \epsilon)\,[1 + O(\epsilon^{-m})] \tag{6.43}$$

for arbitrary m.

Asymptotic Evaluation of $\vec{\theta}$

We now turn to our main task of obtaining an asymptotically valid expression for $\vec{\theta}$ for the specialized turning point under consideration. Again we return to the specific case of a $c_o^2\eta$ profile having a single maximum (profile M). It is seen, then, that the function $\ell_0(x)$, Eq. (6.7), has a minimum, whence in Eq. (6.26) and the following discussion, $\delta = i$.

Now corresponding to each of our solutions $\vec{\psi}_\nu$, Eq. (6.43), of Eq. (6.11) we have, by the latter equation, a solution $\vec{\theta}_\nu$ of the original Eq. (6.3). For large ϵ, it is seen from Eq. (6.9), (6.8), and (6.5) that only the transformation $\underset{\sim}{S}_0$ is important, and we obtain

$$\vec{\theta}_\nu \sim \underset{\sim}{Q}_0 \cdot \vec{\psi}_\nu \exp \int_0^x [\tfrac{1}{2}\epsilon(\mu_1 + \mu_2) + g_0]\, dx' \tag{6.44}$$

for all x.

To find $\vec{\theta}$ asymptotically, we require the particular $\vec{\theta}_\nu$, Eq. (6.44), which remains bounded as $x \to \infty$. We contend that $\vec{\theta}_1$, in fact, satisfies this condition; for, writing out the latter explicitly, using $\underset{\sim}{Q}_0$ from Appendix C and $\vec{\psi}_1 \sim \vec{y}^{(0)}$ from Eq. (6.40), we have

$$\begin{aligned}\vec{\theta}_1(x, \epsilon) \sim & - \phi(z)^{-\frac{1}{2}} (\underset{\sim}{T} \cdot \hat{e}_1)(2i\epsilon)^{k-\frac{1}{4}} \left[\int_0^z \phi(z')dz'\right]^k \\ & \exp\left\{\int_0^x [\tfrac{1}{2}\epsilon(\mu_1 + \mu_2) + g_0]dx' + \int_0^z \left[- i\epsilon\phi(z') \right.\right. \\ & \left.\left. - \frac{p_1(z') - p_1(0)\Pi^4(0)/\Pi^4(z')}{2\phi(z')}\right]dz' \right\},\end{aligned} \tag{6.45}$$

where $\underset{\sim}{T}$ is the transform matrix Eq. (3.1) and where the variable $z = x - x^*$ must be carefully distinguished from x. Since for $x > x^*$, $\phi(z)$, Eq. (6.26) and (6.7), is the real positive quantity

$$\phi(z) = p_0^{\frac{1}{2}} = - \frac{i\mu_{21}}{2}, \quad x > x^* \tag{6.46}$$

we see that the ϵ term in the exponential is

$$\int_0^x \mu_1 dx' + \int_0^{x^*} \tfrac{1}{2}\mu_{21} dx'. \tag{6.47}$$

Thus, $\vec{\theta}_1$ is of the μ_1 type in the sense of Sec. 3. Bringing the function of x, other than $(\underset{\sim}{T} \cdot \hat{e}_1)$, into the exponential, we obtain the ϵ-independent part of the latter to be

$$\int_0^x g_0(x')dx' - i\int_0^z \frac{\ell_1(x^*+z') - \ell_1(x^*)\Pi^4(0)\phi^2(z')/\int_0^{z'}\phi(z'')dz''}{2\phi(z')}dz'$$

$$+\int_{z_0}^{z}\left[k_0\frac{\phi(z')}{\int_0^{z'}\phi(z'')dz''} - \tfrac{1}{2}\frac{d\ \ell n\ \phi}{dz'}\right]dz' \qquad (6.48)$$

where the point z_0 is an arbitrary positive number. Now by Eq. (6.29d) and (6.26)

$$k_0 = -\tfrac{1}{2}\, i\ell_1(x^*)\Pi^4(0) \qquad (6.49)$$

while from Appendix C, Eq. (C.8), (C.19), and (C.20),

$$\ell_1(x) = \frac{\kappa s}{\eta u}(E_{11} - E_{22})$$

$$g_0(x) = \tfrac{1}{2}\left[E_{11} + E_{22} + \frac{d\ \ell n}{dx}\left(\frac{\kappa s}{\eta u}\right)\right], \qquad (6.50)$$

whence it follows that Eq. (6.48) has as its x derivative E_{11}, as in the asymptotic expression (3.3), as seen in Eq. (3.6). (This is, of course, a necessary conclusion since the present asymptotic expressions must agree with those of Sec. 3 away from the turning point.) Therefore, the present $\vec{\theta}_1$ is, outside of a multiplicative factor, identical with $\vec{\theta}_1$ of Sections 3 and 4, and we have, as in Eq. (4.6),

$$\vec{\theta}(x, \epsilon) \sim \vec{\theta}_1(x, \epsilon), \tag{6.51}$$

but now without restriction on x.

The solution for $x < x^*$ is, therefore, given through Eq. (6.40b) to be

$$\vec{\theta}_1(x, \epsilon) \sim \left\{ - \frac{2\pi i e^{2k\pi i}}{\Gamma(\frac{1}{4}-k)\Gamma(3/4-k)} (2i\epsilon)^{-k-\frac{1}{4}} \left[\int_0^z \phi(z')dz' \right]^{-k} (\underset{\sim}{T} \cdot \hat{e}_1) \right.$$

$$e^{\frac{1}{2}\psi+j} + e^{-4k\pi i}(2i\epsilon)^{k-\frac{1}{4}} \left[\int_0^z \phi(z')dz' \right]^{k} (\underset{\sim}{T} \cdot \hat{e}_2) \tag{6.52}$$

$$\left. e^{-(\frac{1}{2}\psi+j)} \right\} \frac{\exp\left\{ \int_0^x [\frac{1}{2}\epsilon(\mu_1+\mu_2) + g_0]dx' \right\}}{\phi(z)^{\frac{1}{2}}} .$$

Since, for $x < x^*$, $\phi(z)$ is the negative real quantity,

$$\phi(z) = p_0^{\frac{1}{2}} = \tfrac{1}{2}i\mu_{21} , \qquad x < x^* \tag{6.53}$$

the first contribution to Eq. (6.52) is of the μ_1 type and the second of the μ_2 type. If we rescale $\vec{\theta}$ so that the μ_1-type contribution is simply $\underset{\sim}{T} \cdot \hat{e}_1$ for $x = 0$, we can write for $x < x^*$

$$\vec{\theta}(x, \epsilon) \sim (\underset{\sim}{T} \cdot \hat{e}_1) \exp \int_0^x (\epsilon\mu_1 + E_{11})dx'$$

$$+ \alpha(\epsilon, \upsilon)(\underset{\sim}{T} \cdot \hat{e}_2) \exp \int_0^x (\epsilon\mu_2 + E_{22})dx' \tag{6.54}$$

$$\alpha(\epsilon, \upsilon) = \left[- 2i\epsilon \int_0^{-x^*} \phi(z')dz' \right]^{2k_0} \frac{\Gamma(\frac{1}{4}-k_0)\Gamma(3/4-k_0)}{2\pi i \exp(6k_0\pi i)} \exp \int_0^{x^*} (\epsilon\mu_{12} + X_{12})dx'$$

$$X_{12} = \frac{\ell_1(x^*+z) - \ell_1(x^*)\Pi^4(0)/\Pi^4(z)}{\phi(z)} .$$

This is precisely of the form of Eq. (4.24) for all other Class II values of ζ_i for profile M, but with a redetermination of α.

Now the expression for $V(\tau, \epsilon)$ (whose zeros determine stability) is to be obtained from Eq. (6.54) and (6.45) (the latter must first be rescaled as above, of course) by following again the procedure of Sec. 5. It follows once more that the final asymptotic expression is given by Eq. (5.17) and we turn now to consider the nature of α at the current value of ζ. However, there is no need to locate the roots of L, as will be seen by considering the magnitude of $\alpha(\epsilon, \upsilon)$.

Since μ_{12} is pure imaginary, $|\alpha|$, in its dependence of ϵ, is seen from Eq. (6.54) to be given by the factor ϵ^{2k_0}. One finds for k_0, Eq. (6.49), using Eq. (6.28),

$$k_0 = - \ell_1(x^*)/4\phi'(0) \tag{6.55}$$

and using Eq. (6.50) and the values of E_{11} and E_{22} from Appendix A, this becomes

$$k_0 = k_{00} - \upsilon k_{01}$$

$$k_{00} = -\frac{\zeta_i}{4\phi'(0)\eta u}\left\{\left[\frac{(1-\eta)vp_S}{T} - \frac{2u^2}{u^2+\zeta_i^2}\right]\frac{\vec{\sigma}\cdot\vec{r}}{\eta u}\right.$$

$$\left. + \frac{(1-\eta)\vec{\sigma}\cdot\vec{r}_v}{\eta m} - \frac{d\ \ell n\ \eta}{dx}\right\}_{x=x^*} \tag{6.56}$$

$$k_{01} = \frac{\zeta_i}{4\phi'(0)}\left[\frac{2(1-\eta)}{u^2\eta^2}\right]_{x=x^*}.$$

Since k_{01} is positive, $\mathrm{Re}(k_0)$ is clearly negative, provided υ satisfies

$$\mathrm{Re}(\upsilon) > \max\ (0,\ k_{00}/k_{01}). \tag{6.57}$$

For such υ, then, α vanishes in the limit and only the μ_1-type solution contributes to $\vec{\theta}$ asymptotically. If, however, $k_{00} > 0$, then in the range

$$0 \le \mathrm{Re}(\upsilon) < k_{00}/k_{01}, \tag{6.58}$$

α becomes infinite. In the expressions for $\vec{\theta}$ and L, the μ_2-type solution dominates in the $\epsilon \to \infty$ limit. This behavior is just that predicted for profile M previously; for it is readily seen from Eq. (5.18) that, if k_0 is positive, then β_2 (in the Sec. 5 expression for α) for ζ_i near $i(c_o\eta^{\frac{1}{2}})_{max}$ is large and positive. Hence, the μ_2-type contribution also dominates for ζ_i just below the special value of ζ_i. Similarly, if k_0 is

negative, then β_2 is large and negative and the μ_1-type contribution dominates. In view of the criterion for instability arrived at in Sec. 5, viz. Eq. (5.20), the criterion for instability at the present special value of ζ_i is the inequality

$$k_{00} > 0 \tag{6.59}$$

which is a purely algebraic condition on the equation of state and the chemical kinetics, as opposed to the integral condition, Eq. (5.20).

Continuity of the Asymptotic Solution for Profile M

Having arrived now at a stability criterion for all Class III values of ζ, we have completed the treatment of profile M, except that we still have not demonstrated that the asymptotic expression for $V(\tau, \epsilon)$ behaves continuously with $\tau = \epsilon\zeta + \upsilon$ through the point $\zeta = i(c_o\eta^{\frac{1}{2}})_{max}$. In terms of $\vec{\theta}$, the continuity of V requires that for $x = 0$ the $\vec{\theta}_2$ contribution should vanish when ζ passes from Class III to Class I; for we recall from Sec. 4 that for ζ in Class I there is no $\vec{\theta}_2$ contribution.

From the discussion of the magnitude of $\alpha(\epsilon, \upsilon)$, it is evident that in the stable case ($k_{00} < 0$), the $\vec{\theta}_2$ contribution does vanish continuously with ζ_i since $\alpha(\epsilon, \zeta, \upsilon)$, Eq. (5.18), approaches zero at $\zeta_i = (c_o\eta^{\frac{1}{2}})_{max}$. In the unstable case, however, it is clear that the $\vec{\theta}_2$ contribution vanishes discontinuously with ζ at this special value $i(c_o\eta^{\frac{1}{2}})_{max}$, if $Re(\upsilon)$ lies in the range Eq. (6.58). We now will

demonstrate that, for less "violent" changes of $\tau = \epsilon\zeta + \upsilon$ (i.e., changes of υ rather than ζ), the $\vec{\theta}_2$ contribution also vanishes continuously.

Now we have already seen that by increasing $\mathrm{Re}(\upsilon)$ through the value k_{00}/k_{01} [see Eq. (6.58)], the desired effect takes place. Similarly for $\mathrm{Re}(\upsilon) < k_{00}/k_{01}$, we will now show that the magnitude of α diminishes with increasing $\mathrm{Im}(\upsilon)$ and that continuity holds in this direction in the τ-plane. To study the magnitude of $\alpha(\epsilon, \upsilon)$, Eq. (6.54), with variations of $\mathrm{Im}(\upsilon)$, we first employ the Legendre-Gauss multiplication theorem[24] to write

$$\Gamma(\tfrac{1}{4} - k_0)\ \Gamma(3/4 - k_0) = \Gamma(\tfrac{1}{2} - 2k_0)\pi^{\frac{1}{2}}2^{2k_0+\frac{1}{2}} .$$

Consider now the magnitude of α for <u>both</u> ϵ and $\mathrm{Im}(\upsilon) = \upsilon_i$ large; using the above identity with Eq. (6.54), we obtain

$$|\alpha(\epsilon, \upsilon)| = K_0\Gamma(\tfrac{1}{2} - 2k_0)\ \exp\ [2k_0\ \ell n\ \epsilon - 5k_{01}\pi\upsilon_i] \qquad (6.60)$$

with K_0 composed of various factors independent of υ_i and ϵ. The gamma function is given asymptotically in υ_i by the formula[25]

$$|\Gamma[\tfrac{1}{2} - 2\ \mathrm{Re}(k_0) + 2ik_{01}\upsilon_i]| \sim K_1\ \exp\ [-\ 2\ \mathrm{Re}(k_0)\ \ell n\ \upsilon_i - k_{01}\pi\upsilon_i]$$

with K_1 representing a constant. Combining this with Eq. (6.60), we see that $|\alpha|$ becomes small for υ_i of order of $\ell n\ \epsilon$, i.e.,

$$\upsilon_i > \upsilon_{ic}$$

$$\upsilon_{ic} = K_2\ \ell n\ \epsilon\ . \qquad (6.61)$$

The continuity of the asymptotic theory for profile M is, then, established.

7. A → B DETONATIONS

The preceding theory is here applied to the idealized, one-reaction A → B detonations, having Arrhenius rate constant.[4] The equations for the steady flow are given in Ref. 4 and are repeated here only in so far as required. The notation of that article is slightly modified here; we note particularly that in the present notation the Mach number of the shock is κ_- (rather than κ, which we use here for the local Mach number) and that the frozen sound speed is c_o (rather than c), so that the frozen sound speed in the quiescent gas is c_{o-} (rather than c_o).

Profiles of $c_o^2\eta$

One readily computes this quantity in terms of the mole fraction λ of reactant A to be

$$c_o^2\eta = \frac{u_+^2\omega(\gamma_o+1)}{(1-\omega)^2}(1 - \omega\xi)\xi$$

$$\xi^2(\lambda) = 1 - (1 - \lambda)\, Q/\Omega \qquad (7.1)$$

$$\omega = (\kappa_-^2 - 1)/(\gamma_o\kappa_-^2 + 1)$$

$$\Omega = \gamma_o(\kappa_-^2 - 1)^2/2(\gamma_o^2 - 1)\kappa_-^2$$

where Q is the heat of reaction in units of RT_-, and where ξ varies between 1 at the shock to some equilibrium value $\xi_e \geq 0$. Since λ decreases to zero monotonically according to the Arrhenius rate law

$$d\lambda/dt = - \hat{k}\lambda \exp(-E^{\ddagger}/RT) \tag{7.2}$$

(where $\hat{k}$, the pre-exponential factor, and $E^{\ddagger}$, the activation energy, are constants), the derivative of $c_o^2\eta$ with respect to x has the sign of $(2\omega\xi - 1)$.

A particularly simple case arises if the ratio of (frozen) specific heats γ_o is taken greater than 2, for then $(2\omega\xi - 1)$ is readily seen to be negative for $\xi = 1$ and hence for all $0 \leq \lambda \leq 1$, irrespective of detonation velocity and irrespective of heat of reaction. In this case, all detonations exhibit profile D and are stable asymptotically in ϵ.

For $1 < \gamma_o < 2$, we examine $2\omega\xi - 1$ at the shock ($\xi = 1$) and find it to be positive unless

$$\kappa_-^2 < 3/(2 - \gamma_o).$$

For "normal" values of γ_o, i.e., less than the ideal-monatomic-gas value of 5/3, it is not expected that detonations will have such small velocities, but for sufficiently small heats of reaction, viz.

$$Q < \tilde{Q}(\gamma_o)$$

$$\tilde{Q}(\gamma_o) = \gamma_o(\gamma_o + 1)/6(2 - \gamma_o)(\gamma_o - 1), \tag{7.3}$$

the CJ Mach number

$$\kappa_{-CJ}^2 = 1 + h\,(1 + \tfrac{1}{4}h^2)^{\frac{1}{2}} + \tfrac{1}{2}h^2$$

$$h^2 = 2(\gamma_o^2 - 1)Q/\gamma_o \qquad (7.4)$$

is less than $3/(2 - \gamma_o)$. Thus the situation for $Q < \tilde{Q}$ is that, for $\kappa_-^2 < 3/(2 - \gamma_o)$, $c_o^2\eta$ decreases with distance at the shock and throughout the reaction zone and exhibits profile D once more.

For $\kappa_-^2 > 3/(2 - \gamma_o)$, $c_o^2\eta$ is increasing at the shock, but not necessarily throughout the reaction zone. Since ξ is monotone-increasing in λ (which decreases with x) and since $(2\omega\xi - 1)$ is monotone-increasing in ξ, it is seen that $c_o^2\eta$ has at most a single maximum. Now the value of $(2\omega\xi - 1)$ at equilibrium is negative for the CJ detonation (for ξ vanishes at $\lambda = 0$ in this case) but becomes positive for sufficient overdrive since, by Eq. (7.1), ξ remains unity throughout the reaction zone in the limit $\kappa_- \to \infty$. There exists, therefore, a transitional Mach number κ_{-t} above which $(2\omega\xi - 1)$ is positive throughout the detonation. One finds

$$\kappa_{-t}^2 = \frac{2}{4-\gamma_o^2}\left\{ h^2 + \frac{4+\gamma_o}{2} + \left[\left(h^2 + \frac{4+\gamma_o}{2}\right)^2 - \frac{3(4-\gamma_o^2)}{4}\right]^{\frac{1}{2}} \right\}. \qquad (7.5)$$

The behavior of $c_o^2\eta$ is summarized in Table III for all values of the parameters. It should be remembered that the possibility of instability is limited to profiles I and M.

TABLE III

Classification of the profile of $c_o^2\eta$ versus distance x in the steady detonation, according the types in Fig. 5, for the A → B idealized detonation.

Heat capacity ratio, γ_o	Reduced heat of reaction, Q	Mach number of detonation, κ_-	Profile
> 2	all	all	D
< 2	$< \mathcal{Q}(\gamma_o)$	$\kappa_{-CJ}^2 \leq \kappa_-^2 < 3/(2 - \gamma_o)$	D
		$3/(2 - \gamma_o) \leq \kappa_-^2 < \kappa_{-t}^2$	M
		$\kappa_{-t}^2 \leq \kappa_-^2$	I
	$< \mathcal{Q}(\gamma_o)$	$\kappa_{-CJ}^2 \leq \kappa_-^2 < \kappa_{-t}^2$	M
		$\kappa_{-t}^2 \leq \kappa_{-t}^2$	I

General Considerations of the Stability Criterion

The implications of the asymptotic theory can be found by the evaluation of exp (β_2) and L_1/L_2 for Class III values of ζ, for specific values of the reduced heat of reaction Q, the reduced activation energy $Q^\ddagger = E^\ddagger/RT_-$, the heat capacity ratio γ_o, and the degree of overdrive $f = \kappa_-^2/\kappa_{-CJ}^2$. If we denote the value of $\xi(\lambda)$, Eq. (7.1), at the turning point x* by ξ^*, then the correspondence between ζ_i and ξ^* is

$$\zeta_i^2 = u_+^2 \omega(\gamma_o + 1)(1 - \omega\xi^*)\xi^*/(1 - \omega)^2 . \qquad (7.6)$$

Transformation of Eq. (5.18) to the variable

$$\tilde{z}(\xi) = [(1 - \omega\xi^*)\xi^* - (1 - \omega\xi)\xi]^{\frac{1}{2}} \qquad (7.7)$$

yields for β_2, after substitution from Eq. (7.1) and (7.2),

$$\beta_2(\zeta_i) = 2\omega[(1 - \omega\xi^*)\xi^*]^{\frac{1}{2}} \int_0^{\tilde{z}(1)} I_2(\tilde{z})d\tilde{z}$$

$$I_2(\tilde{z}) = [(1 - \omega\xi)(1 + \omega\gamma_o\xi)]^{-\frac{1}{2}}(2\omega\xi - 1)^{-1}K(\tilde{z}) \qquad (7.8)$$

$$K(\tilde{z}) = (\gamma_o - 1)\left(\frac{E^\ddagger}{RT} - 1\right) - \frac{1}{\omega\xi} + \frac{2(1+\omega\gamma_o\xi)(1-\omega\xi)}{(1-\omega\xi)^2+\omega(\gamma_o+1)(1-\omega\xi^*)\xi^*} .$$

$$\xi(\tilde{z}) = (2\omega)^{-1}\left\{1 + [1 - 4\omega(1 - \omega\xi^*)\xi^* + 4\omega\tilde{z}^2]^{\frac{1}{2}}\right\} .$$

The activation energy term is given by

$$\frac{E^\ddagger}{RT} = \frac{(\gamma_o+1)^2\kappa^2}{(\gamma_o\kappa^2+1)^2} Q^\ddagger[1 + \omega\gamma_o\xi)(1 - \omega\xi)]^{-1} . \qquad (7.9)$$

Now it is evident that β_2 becomes large and positive for large activation energy and, in fact, becomes linear in $Q^\ddagger$. For any ζ_i for which L_2 is non-zero, it follows that the detonation becomes unstable for all sufficiently large activation energies. On the other hand, it can be shown that for all sufficiently large detonation velocities

$$|L_1/L_2| > \exp(\beta_2) ,$$

and hence detonations are stable for large values of f.

In addition, a sufficient condition for instability can be derived by a comparison of the derivatives of $\exp(\beta_2)$ and L_1/L_2 at $\zeta_i = (c_o \eta^{\frac{1}{2}})_+$. The derivatives with respect to ζ_i itself do not exist, but we have

$$\left[\frac{d\beta_2}{d\tilde{z}(1)}\right]_{\tilde{z}(1)=0} = \frac{2\omega}{(2\omega-1)(1-\omega\gamma_o)^{\frac{1}{2}}}\left[(\gamma_o - 1)\left(\frac{E^\ddagger}{RT_+} - 1\right) + \frac{2\omega-1}{\omega}\right]$$

$$\left[\frac{dL_1/L_2}{d\tilde{z}(1)}\right]_{\tilde{z}(1)=0} = \frac{4\kappa_-^2}{(1+\omega\gamma_o)^{\frac{1}{2}}} \qquad (7.10)$$

where $\tilde{z}(1)$ is given by Eq. (7.7). If the former exceeds the latter, the $\exp(\beta_2)$ curve leaves the value 1 at the left in Fig. 7 above the L_1/L_2 curve, whence the flow is unstable. The neutral stability point with respect to this condition yields a transitional activation energy $Q_t^\ddagger$ for each Mach number

$$Q_t^\ddagger(\kappa_-^2) = \frac{T_+}{T_-}\left[1 + \frac{(2\omega-1)(2\kappa_-^2-1)}{\omega(\gamma_o-1)}\right] \qquad (7.11)$$

which is independent of Q. For $Q^\ddagger > Q_t^\ddagger$, the flow is unstable, while, for $Q^\ddagger < Q_t^\ddagger$, the $\exp(\beta_2)$ curve begins below the L_1/L_2 curve. For fixed values of Q and γ_o, the value of $Q^\ddagger$ below which the latter situation [with regard to $\exp(\beta_2)$ and L_1/L_2] holds for <u>all</u> detonation velocities is evidently given by the minimum of $Q_t^\ddagger$. Now the minimum of $Q_t^\ddagger$ (for profiles I and M) occurs at the smallest detonation velocity. Thus, for

$Q < \tilde{Q}$, the minimum is at the profile D-M transition, where

$$Q^{\ddagger}_{tm} = Q^{\ddagger}_{t}[3/(2 - \gamma_o)] = \frac{2+\gamma_o}{3(2-\gamma_o)} \text{ , for } Q < \tilde{Q} \text{ .} \tag{7.12a}$$

and, for $Q > \tilde{Q}$, at the CJ detonation velocity,

$$Q^{\ddagger}_{tm} = Q^{\ddagger}_{t}(\kappa^2_{-CJ}), \text{ for } Q > \tilde{Q} \text{ .} \tag{7.12b}$$

In order that a system with given Q and γ_o be asymptotically stable for all detonation velocities, it is, therefore, necessary that $Q^{\ddagger} < Q^{\ddagger}_{tm}$.

Numerical Results

An IBM-7094 computer was programmed to evaluate β_2, L_1, and L_2 throughout the turning-point region

$$(c_o\eta^{\frac{1}{2}})_+ < \zeta_i < (c_o\eta^{\frac{1}{2}})_{max}$$

for specified values of the parameters Q, $Q^{\ddagger}$, f, and γ_o. For $\kappa^2_- < \kappa^2_{-t}$, the value of k_{00}, Eq. (6.56), was also evaluated for $\zeta_i = (c_o\eta^{\frac{1}{2}})_{max}$ in order to ascertain stability at the maximum of profile M. A plot of $\exp(\beta_2)$ and $|L_1/L_2|$ as functions of ζ_i, as discussed in Sec. 5 in connection with Fig. 7, demonstrates instability by the presence of a region for which the exponential lies above the $|L_1/L_2|$ curve. It is to be noted, however, that, in the absence of a back reaction (B → A), $\beta_2(\zeta_i)$ does not approach $-\infty$ as $\zeta_i \to (c_o\eta^{\frac{1}{2}})_{x=\infty}$, but attains a finite value, as seen from Eq. (7.8). This value of ζ_i (corresponding to the turning point being at $x = \infty$) is characterized by a discontinuous behavior of $\vec{\theta}$ and V, much like that previously discussed for profile M.

Inasmuch as this phenomenon is purely a result of the reaction model, there seems to be no compulsion to investigate it further.

The results of our numerical analysis for $\gamma_o = 1.2$ can best be shown in the form of the neutral stability curves in the (Q, f)-plane. In Fig. 8 are shown these curves for the activation energies of $Q^\ddagger = 50$ and $Q^\ddagger = 10$. It is seen from Eq. (7.12) that, in both instances, the profile-D-to-profile-M transition locus, viz., $\kappa_-^2 = 3.75$, is also a neutral stability locus. The rightmost neutral stability curve has a more complex structure for $Q^\ddagger = 50$. The lower section, i.e., the portion below $Q \approx 1$, corresponds within numerical error to the constant Mach number root of Eq. (7.11) for $Q_t^\ddagger = 50$, namely, $\kappa_-^2 = 7.084$. In the unstable region to the left of $\kappa_-^2 = 7.084$, the exp (β_2) curve "begins" above the $|L_1/L_2|$ curve, but for some $\zeta_i = \zeta_{i2}$ falls below the latter, as in Fig. 7. With increasing f, ζ_{i2} is found to decrease, apparently merging with $\zeta_{i1} = (c_o \eta^{\frac{1}{2}})_+$ at $\kappa_-^2 = 7.084$.

The upper section of the rightmost neutrally stability curve does not correspond to the necessary condition, Eq. (7.11). For fixed Q above $Q \approx 1$, the exp (β_2) "begins" below the $|L_1/L_2|$ curve when $\kappa_-^2 > 7.084$, but for the range, $\zeta_{i1} < \zeta_i \leq (c_o \eta^{\frac{1}{2}})_{x=\infty}$, lies above the $|L_1/L_2|$ curve. These ζ_i are then unstable, but, with increasing detonation velocity, the unstable range of ζ_i decreases [i.e., ζ_{i1} approaches $(c_o \eta^{\frac{1}{2}})_{x=\infty}$], finally vanishing (at the neutrally stable value of f) with $\zeta_{i1} = (c_o \eta^{\frac{1}{2}})_{x=\infty}$.

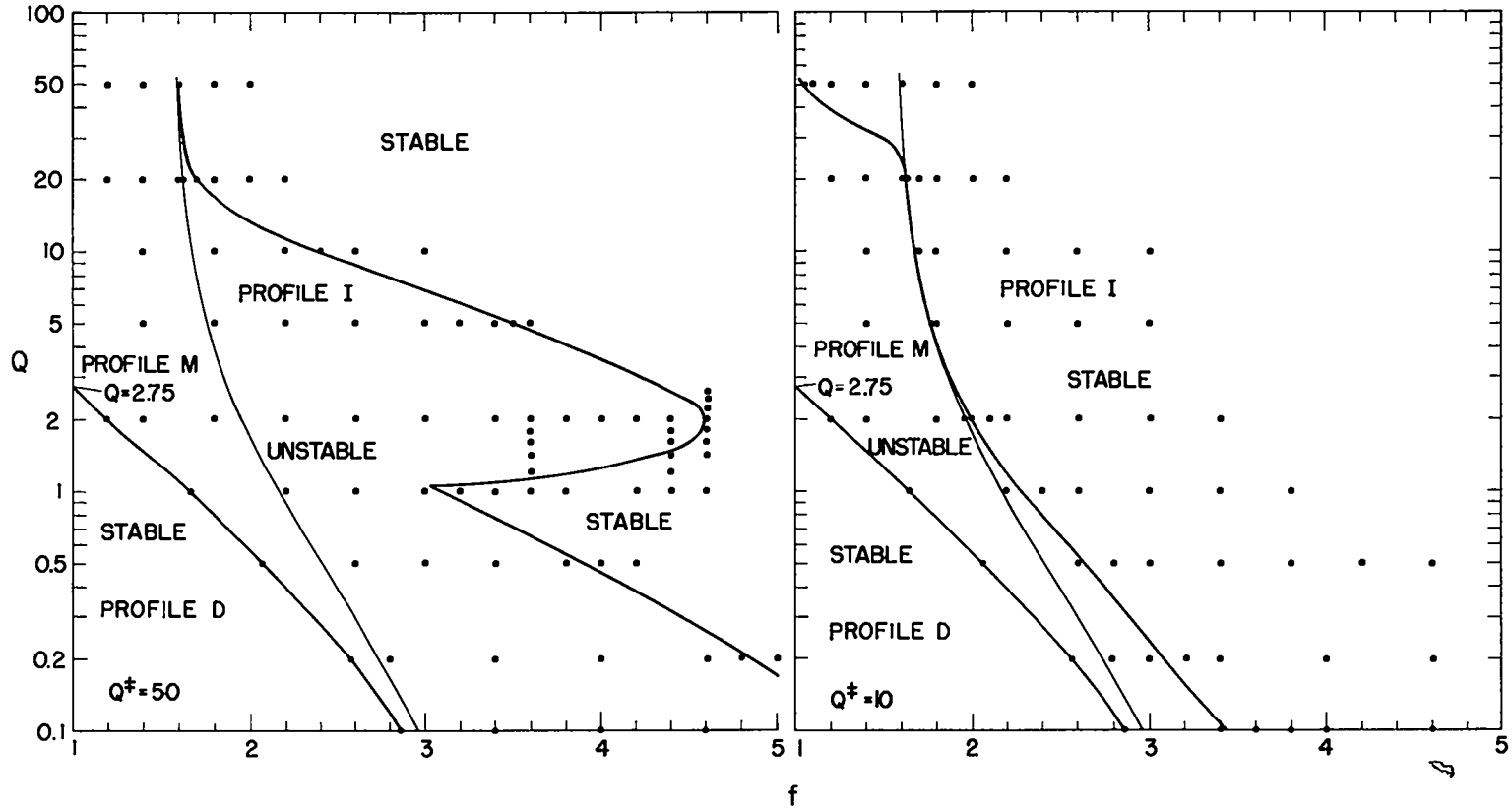

Fig. 8 Stability in the limit of vanishing transverse wavelength for a heat capacity ratio $\gamma_o = 1.2$ and reduced activation energies of (a) $Q^\ddagger = 50$ and (b) $Q^\ddagger = 10$ for various values of the reduced heat of reaction Q and degree of overdrive $f = (\kappa_-/\kappa_{-CJ})^2$. The light curve is the transition locus from profile M to profile I (see Fig. 5). The heavy curves are neutral stability curves, the leftmost of these also being the profile-D-to-profile-M transition locus, $\kappa_-^2 = 3/(2 - \gamma_o)$. The dots indicate the values for which the calculation has been performed.

For the smaller activation energy, $Q^{\ddagger} = 10$, the unstable regime is considerably smaller, and the rightmost neutral stability locus lies to the right of the root of Eq. (7.11) for $Q_t^{\ddagger} = 10$, at least for $Q \geq 0.5$ and lies very near to this root for $Q < 0.5$. If a "bulge" of the type seen for $Q^{\ddagger} = 50$ exists, it is very small in this case. It should also be noted in connection with the $Q^{\ddagger} = 10$ results that the previous long-wavelength calculations[4] found instability in regions of asymptotic stability. Thus, the $Q = 50$ detonations were previously found to be unstable, apparently for all degrees of overdrive while the asymptotic theory predicts stability for all $f > 1.04$.

The most astonishing feature of Fig. 8 is the presence of instability for a range of f values at <u>all positive heats of reaction.</u> This feature was not present in the long-wavelength calculations[4] but its correctness is indicated by the fact that we have been able to calculate an unstable root for $Q = 0.1$, $f = 4.0$ by means of the numerical program described in Ref. 4. This program is ineffective for large values of ϵ by virtue of the inability of the program to integrate the $\vec{\theta}$ differential equation when the magnitude of the eigenvalue (having negative real part) of $-\underset{\sim}{P}'(\infty, \tau, \epsilon)$, Eq. (2.4), is large. This is the case for large ϵ, except in the turning-point region of the τ-plane. Therefore, by computing β_1 and β_3 as well as β_2, L_1 and L_2 for a particular value of ζ_i for which the condition for instability holds, we find a root of the asymptotic expression $L_1 + \alpha L_2$ to occur at the point, [see Eq. (5.18)]

$$\mathrm{Re}(\upsilon) = \frac{\beta_2(\zeta_i) - \ell n\ |L_1(i\zeta_i)/L_2(i\zeta_i)\ |}{\beta_3(\zeta_i)}$$

$$\epsilon = \begin{cases} 3\pi/2\beta_1(\zeta_i), & \text{for } L_2(i\zeta_i) > 0 \\ \pi/2\beta_i(\zeta_i), & \text{for } L_2(i\zeta_i) < 0 \end{cases} \qquad (7.13)$$

$$\mathrm{Im}(\tau) = \epsilon\zeta_i \ .$$

For $\zeta_i = 1.752818\ u_+$, we obtained the asymptotic root

$$\epsilon = 15.77321$$
$$\tau = \ 0.001811 + i\ 27.53626. \qquad (7.14)$$

We have also determined an "exact" root of $V(\tau, \epsilon)$ for this value of ϵ by determining V, by means of the numerical calculation of Ref. 4, for an array of values of τ near the predicted root. Interpolation yields the root,

$$\tau = 0.0021383 + i\ 27.536277. \qquad (7.15)$$

The units of length and time for $1/\epsilon$ and $1/\tau$, respectively, are the distance and time to half-reaction, as in Ref. 4. The accuracy of the "exact" result cannot be expected to exceed the third digit to the right of the decimal point.

The transition to stability for all Q and f has not been intensively investigated; but for $Q^{\ddagger} < 4/3$, it follows from Eq. (7.12) that the <u>sufficient</u> condition for <u>instability</u> is not satisfied,

irrespective of Q and f. Numerical evidence suggests that, as the activation energy approaches $Q^{\ddagger} = 4/3$ from above, the rightmost neutral stability curve approaches the profile D-M transition locus. Hence for $Q^{\ddagger} < 4/3$ it is believed that all detonations in this system are stable for small transverse wavelengths. No attempt to prove this conjecture has been made, but it has been proved to be at least approximately true.

One final point seems worth mentioning, namely the approach to Q = 0, the step shock. The exact expression for $V(\tau, \epsilon)$ is known for the step shock, of course, namely

$$V = \epsilon L_1(\zeta),$$

and this has no roots on the imaginary ζ axis. As described above in conjunction with Fig. 8, the asymptotic theory formally predicts for Q = 0 a range of unstable shock velocities, dependent upon the activation energy, $Q^{\ddagger} > 4/3$. In the Q = 0 limit, however, it can readily be shown that $\beta_1 \to 0$ and $\beta_3 \to \infty$. Thus, according to Eq. (7.13), the rate of growth of the predicted "instability" is zero while the wavelength vanishes. Thus, while the asymptotic theory is not exactly continuous at the Q = 0 point, it does not predict an incorrect result.

8. DISCUSSION

It is clear from the numerical results for the idealized system that the asymptotic theory provides considerable additional information on the behavior of detonations and obviously should be an integral part

of any stability calculation. In addition, the possibility that rather small-scale transverse disturbances [the wavelength of the root, Eq. (7.15), is about 0.1 in units of the distance to 95% complete reaction] are unstable, even though long wavelengths are stable, is certainly not contrary to experimental evidence. The latter seems to indicate the presence of small-scale, transverse inhomogeneities even when the conditions are well removed from those associated with spin.

Although the present theory does not completely describe the stability behavior of a detonation, it does, nonetheless, provide a computationally simple criterion, the fulfillment of which is a sufficient condition for the growth of disturbances. The application of the present theory would appear to be entirely feasible, irrespective of the number of chemical reactions and the complexity of the equation of state; in this respect, it might well represent the only theoretical test of stability which is available.

In connection with two- or three-dimensional calculations of time-dependent, reactive flows (should such ever become feasible), the presence of asymptotic instability has the greatest importance. In a calculation involving no transport effects, continued refinement of the mesh would evidently increase the number of permitted unstable modes, and a mesh extrapolation would apparently be meaningless. A realistic inclusion of viscosity presumably would be required.

APPENDIX A

The matrices $\underset{\sim}{A}_x$, $\underset{\sim}{A}_y$, and $\underset{\sim}{B}$ are given in Ref. 3 in terms of functions of the state variables in the steady flow. The inverse of $\underset{\sim}{A}_x$ is readily found to be

$$\underset{\sim}{A}_x^{-1} = \frac{1}{u}\begin{bmatrix} -\frac{1-\eta}{\eta} & -\frac{1-\eta}{\eta m} & 0 & \frac{(1-\eta)p_S}{\eta m^2} & \frac{(1-\eta)p_{\vec{\lambda}}}{\eta m^2} \\ -\frac{m}{\eta} & -\frac{1-\eta}{\eta} & 0 & \frac{(1-\eta)p_S}{\eta m} & \frac{(1-\eta)p_{\vec{\lambda}}}{\eta m} \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & \underset{\sim}{I}_n \end{bmatrix} \qquad \text{(A.1)}$$

where $\underset{\sim}{I}_n$ denotes the unit matrix of order n, m is the mass flux u/v, and p is the pressure. Subscripts S, v, and $\vec{\lambda}$ denote partial derivatives, with the remaining variables of the set held fixed.

The calculation of $\underset{\sim}{\Phi}_0$, Eq. (2.76), involves a matrix product yielding

$$\underset{\sim}{\Phi}_0 = \begin{bmatrix} -\frac{(1-\eta)\zeta}{\eta u} & -\frac{m\zeta}{\eta u} & -\frac{im}{1-\eta} & 0 & 0 \\ -\frac{(1-\eta)\zeta}{\eta m u} & -\frac{(1-\eta)\zeta}{\eta u} & 0 & 0 & 0 \\ \frac{i(1-\eta)}{\eta m} & \frac{i}{\eta} & \frac{\zeta}{u} & 0 & 0 \\ \frac{(1-\eta)p_S\zeta}{\eta m^2 u} & \frac{(1-\eta)p_S\zeta}{\eta m u} & \frac{ip_S}{m} & \frac{\zeta}{u} & 0 \\ \frac{(1-\eta)\vec{p_\lambda}\zeta}{\eta m^2 u} & \frac{(1-\eta)\vec{p_\lambda}\zeta}{\eta m u} & \frac{i\vec{p_\lambda}}{m} & 0 & \frac{\zeta}{u}\underset{\sim}{I}_n \end{bmatrix} \qquad (A.2)$$

The eigenvalue-eigenvector problem,

$$[\underset{\sim}{\Phi}_0 - \mu_i \underset{\sim}{I}] \cdot \vec{T}_i = 0 \qquad (A.3)$$

proceeds by finding the determinant of the coefficient matrix to be

$$\left(\frac{\zeta}{u} - \mu_i\right)^{n+2} \left[\left(\frac{1-\eta}{\eta}\frac{\zeta}{u} + \mu_i\right)^2 - \frac{(1-\eta)\zeta^2}{\eta^2 u} - \frac{1}{\eta}\right] . \qquad (A.4)$$

This has roots as follows:

$$\mu_1 = -\frac{\kappa}{\eta u}[\kappa\zeta + s]$$

$$\mu_2 = -\frac{\kappa}{\eta u}[\kappa\zeta - s] \qquad (A.5)$$

$$\mu_3 = \mu_4 = \cdots = \mu_{n+4} = \zeta/u$$

$$s = [\zeta^2 + c_o^2\eta]^{\frac{1}{2}} .$$

The determination of the corresponding eigenvectors is somewhat laborious but straightforward. The $\vec{T}_i$ form the columns of the matrix

$$\underset{\sim}{T} = \begin{bmatrix} \frac{ms}{\kappa u} & -\frac{ms}{\kappa u} & -\frac{im}{i-\eta} & 0 & 0 \\ \frac{\zeta}{u} & \frac{\zeta}{u} & i & 0 & 0 \\ -i & -i & \frac{\zeta}{u} & 0 & 0 \\ -\frac{\kappa s p_S}{mu} & \frac{\kappa s p_S}{mu} & 0 & 1 & 0 \\ -\frac{\kappa s \vec{p_\lambda}}{mu} & \frac{\kappa s \vec{p_\lambda}}{mu} & 0 & 0 & \underset{\sim}{I}_n \end{bmatrix} \qquad (A.6)$$

which has inverse,

$$\underset{\sim}{T}^{-1} = \begin{bmatrix} \frac{\kappa u}{2ms} & \frac{u}{2s}\frac{\kappa\zeta+s}{\zeta+\kappa s} & \frac{i\eta u^2}{2\kappa s(\zeta+\kappa s)} & 0 & 0 \\ -\frac{\kappa u}{2ms} & -\frac{u}{2s}\frac{\kappa\zeta-s}{\zeta-\kappa s} & -\frac{i\eta u^2}{2\kappa s(\zeta-\kappa s)} & 0 & 0 \\ 0 & \frac{iu^2}{\zeta^2-u^2} & \frac{u\zeta}{\zeta^2-u^2} & 0 & 0 \\ \frac{(1-\eta)p_S}{m^2} & -\frac{u^2 p_S}{m(\zeta^2-u^2)} & \frac{iup_S}{m(\zeta^2-u^2)} & 1 & 0 \\ \frac{(1-\eta)\vec{p_\lambda}}{m^2} & -\frac{u^2 \vec{p_\lambda}}{m(\zeta^2-u^2)} & \frac{iu\vec{p_\lambda}}{m(\zeta^2-u^2)} & 0 & \underset{\sim}{I}_n \end{bmatrix} \qquad (A.7)$$

The calculation of the matrix $\underset{\sim}{E}$, Eq. (3.2) is a laborious procedure, which we now indicate. We had

$$\underset{\sim}{\Phi}_1 = [\underset{\sim}{A}_x^{-1} \cdot (\underset{\sim}{B} + \upsilon \underset{\sim}{I})]'$$

$$= \underset{\sim}{W}_1 + \upsilon(\underset{\sim}{A}_x^{-1})' \qquad (A.8)$$

whence we write

$$\underset{\sim}{E} = \underset{\sim}{E}^{(0)} + \upsilon \underset{\sim}{E}^{(1)}$$

$$\underset{\sim}{E}^{(0)} = \underset{\sim}{T}^{-1} \cdot [\underset{\sim}{W}_1 \cdot \underset{\sim}{T} - d\underset{\sim}{T}/dx] \qquad (A.9)$$

$$\underset{\sim}{E}^{(1)} = \underset{\sim}{T}^{-1} \cdot (\underset{\sim}{A}_x^{-1})' \cdot \underset{\sim}{T}.$$

The matrix $\underset{\sim}{W}_1$ is obtained from Eq. (A.1), and matrix $\underset{\sim}{B}$ is given in Ref. 3 in terms of the gradients in the steady flow and certain rate coefficients. The gradients can be written as products of thermodynamic functions and the chemical rate, so that $\underset{\sim}{B}$ can conveniently be separated into a term linear in the rates and a term linear in the thermodynamic derivatives of the rates. Thus we write

$$\underset{\sim}{B}(x) = \underset{\sim}{B}_0 + \underset{\sim}{B}_1 \qquad (A.10)$$

with $\underset{\sim}{B}_0$ vanishing at equilibrium. Explicitly

$$\underset{\sim}{B}_0 = \begin{bmatrix} -\frac{\vec{\sigma}\cdot\vec{r}}{\eta} & \frac{\vec{\sigma}\cdot\vec{r}}{m\eta} & 0 & 0 & 0 \\ -\frac{m\vec{\sigma}\cdot\vec{r}}{\eta} - \frac{m\vec{r}\cdot\vec{\nabla}\eta}{(1-\eta)^2} & \frac{\vec{\sigma}\cdot\vec{r}}{\eta} & 0 & \frac{\vec{r}\cdot\vec{\nabla}(p_S)}{m} & \frac{\vec{r}\cdot\vec{\nabla}(p_{\vec{\lambda}})}{m} \\ 0 & 0 & 0 & 0 & 0 \\ -\frac{m^2 v\vec{\sigma}\cdot\vec{r}}{(1-\eta)T} & \frac{\vec{\Delta F}\cdot\vec{r}}{uT} & 0 & \frac{\gamma_o v\vec{\sigma}\cdot\vec{r}}{\beta_o T} & \left(\frac{\vec{\Delta F}}{T}\right)_{\vec{\lambda}}\cdot\vec{r} \\ 0 & \frac{\vec{r}}{u} & 0 & 0 & 0 \end{bmatrix} \qquad (A.11)$$

and $\underset{\sim}{B}_1$ has but two non-vanishing rows,

$$\hat{e}_i \cdot \underset{\sim}{B}_1 = 0, \quad i = 1, 2, 3$$

$$\hat{e}_4 \cdot \underset{\sim}{B}_1 = [\vec{r}_v, 0, 0, \vec{r}_S, \vec{r}_{\vec{\lambda}}] \cdot \frac{\vec{\Delta F}}{T} \qquad (A.12)$$

$$\hat{e}_5 \cdot \underset{\sim}{B}_1 = -[\vec{r}_v, 0, 0, \vec{r}_S, \vec{r}_{\vec{\lambda}}] \quad .$$

Here $\vec{\sigma}$ is the important thermodynamic function defined in Ref. 7, $\vec{\nabla}$ is the gradient operator in $\vec{\lambda}$-space, also given in Ref. 7, while subscript $\vec{\lambda}$ denotes the partial thermodynamic derivatives, as previously noted. In addition, we have the following identifications: T is the thermodynamic temperature, γ_o is the usual ratio of frozen specific heats, $\vec{\Delta F}$ is the free energy increment, and β_o is the frozen expansion coefficient

$$\beta_o = (\partial v/\partial T)_{p,\vec{\lambda}}$$

Multiplication by $\underset{\sim}{A}_x^{-1}$, Eq. (A.1) with subsequent transposition yields a corresponding pair of terms,

$$\begin{aligned} \underset{\sim}{W}_1 &= \underset{\sim}{W}_{10} + \underset{\sim}{W}_{11} \\ \underset{\sim}{W}_{10} &= [\underset{\sim}{A}_x^{-1} \cdot \underset{\sim}{B}_0]' \\ \underset{\sim}{W}_{11} &= [\underset{\sim}{A}_x^{-1} \cdot \underset{\sim}{B}_1]' \ . \end{aligned} \tag{A.13}$$

The explicit formulas for each are

$$\underset{\sim}{W}_{10} = \frac{1}{u}\begin{bmatrix} \left[\frac{2(1-\eta)}{\eta} - \frac{vp_S}{T}\right]\frac{\vec{\sigma}\cdot\vec{r}}{\eta} + \frac{\vec{r}\cdot\vec{\nabla}\eta}{\eta(1-\eta)} & \left[\frac{2-\eta}{\eta} - \frac{vp_S}{T}\right]\frac{m\vec{\sigma}\cdot\vec{r}}{\eta} + \frac{m\vec{r}\cdot\vec{\nabla}\eta}{\eta(1-\eta)} & 0 & -\frac{m^2v\vec{\sigma}\cdot\vec{r}}{(1-\eta)T} & 0 \\ -\frac{(2-3\eta)\vec{\sigma}\cdot\vec{r}}{m\eta^2} & -\frac{2(1-\eta)\vec{\sigma}\cdot\vec{r}}{\eta^2} & 0 & -\frac{\vec{\Delta F}\cdot\vec{r}}{uT} & \frac{\vec{r}}{u} \\ 0 & 0 & 0 & 0 & 0 \\ \frac{v\vec{\sigma}\cdot\vec{r}}{\eta c_{vo}} - \frac{(1-\eta)\vec{r}\cdot\vec{\nabla}(p_S)}{\eta m^2} & \frac{u\vec{\sigma}\cdot\vec{r}}{\eta c_{vo}} - \frac{(1-\eta)\vec{r}\cdot\vec{\nabla}(p_S)}{\eta m} & 0 & \frac{\gamma_o v\vec{\sigma}\cdot\vec{r}}{\beta_o T} & 0 \\ -\frac{1-\eta}{\eta m^2}\left[\vec{r}\cdot\vec{\nabla}(p_{\vec{\lambda}}) - p_S\left(\frac{\vec{\Delta F}}{T}\right)_{\vec{\lambda}}\cdot\vec{r}\right] & -\frac{1-\eta}{\eta m}\left[\vec{r}\cdot\vec{\nabla}(p_{\vec{\lambda}}) - p_S\left(\frac{\vec{\Delta F}}{T}\right)_{\vec{\lambda}}\cdot\vec{r}\right] & 0 & \left(\frac{\vec{\Delta F}}{T}\right)_{\vec{\lambda}}\cdot\vec{r} & 0 \end{bmatrix} \tag{A.14}$$

(where c_{vo} is the frozen, constant volume heat capacity); and $\underset{\sim}{W}_{11}$ has three non-vanishing rows,

$$
\begin{aligned}
\hat{e}_i \cdot \underset{\sim}{W}_{11} &= 0, \qquad i = 2, 3 \\
\hat{e}_1 \cdot \underset{\sim}{W}_{11} &= \frac{\vec{r}_v}{u} \cdot \left[-\frac{v\vec{\sigma}}{\eta}, -\frac{u\vec{\sigma}}{\eta}, 0, \frac{\vec{\Delta F}}{T}, \underset{\sim}{I}_n \right] \\
\hat{e}_4 \cdot \underset{\sim}{W}_{11} &= \frac{\vec{r}_S}{u} \cdot \left[-\frac{v\vec{\sigma}}{\eta}, -\frac{u\vec{\sigma}}{\eta}, 0, \frac{\vec{\Delta F}}{T}, \underset{\sim}{I}_n \right] \\
\hat{e}_5 \cdot \underset{\sim}{W}_{11} &= \frac{\vec{r}_\lambda}{u} \cdot \left[-\frac{v\vec{\sigma}}{\eta}, -\frac{u\vec{\sigma}}{\eta}, 0, \frac{\vec{\Delta F}}{T}, \underset{\sim}{I}_n \right] .
\end{aligned}
\tag{A.15}
$$

The calculation of $\underset{\sim}{E}$, Eq. (A.9), involves differentiation of $\underset{\sim}{T}$ as well as matrix multiplications, and we display only the final result for several elements. Thus, we obtain

$$
\begin{aligned}
E_{11}^{(0)} = &- \frac{1-\eta}{2\eta m}\left[\frac{p_S \vec{\sigma}\cdot\vec{r}}{T} + \vec{\sigma}\cdot\vec{r}_v\right] + \frac{2-\eta}{4\eta(1-\eta)}\frac{d\eta}{dx} \\
&+ \frac{\kappa\zeta}{2\eta s}\left[\frac{1}{1-\eta}\frac{d\eta}{dx} - \frac{v p_S \vec{\sigma}\cdot\vec{r}}{Tu} - \frac{\vec{\sigma}\cdot\vec{r}_v}{m}\right] - \tfrac{1}{2}\frac{d\ \ell n\ s}{dx} \\
&+ \frac{\kappa\zeta+s}{\zeta+\kappa s}\frac{\zeta\vec{\sigma}\cdot\vec{r}}{s\eta u}
\end{aligned}
\tag{A.16}
$$

$$
E_{11}^{(1)} = -\frac{\kappa(\zeta+\kappa s)}{u\eta s} \quad .
$$

For E_{22} one obtains a result equivalent to E_{11}, when the square root s is replaced by -s. The off-diagonal elements of $\underset{\sim}{E}$ do not enter into our final discussion in any important way but it is of interest to note that the element

$$E_{21}^{(0)} = -\frac{\vec{\sigma}\cdot\vec{r}}{2\eta u^2}\left[(2-\eta) - \frac{(1-\eta)\eta v p_S}{T}\right] - \frac{2-\eta}{4\eta(1-\eta)}\frac{d\eta}{dx}$$

$$+ \frac{(1-\eta)\vec{\sigma}\cdot\vec{r}_v}{2\eta m} - \frac{\kappa\zeta}{2\eta s}\left[\frac{1}{1-\eta}\frac{d\eta}{dx} + \left(2 - \eta - \frac{\eta v p_S}{T}\right)\frac{\vec{\sigma}\cdot\vec{r}}{\eta u} - \frac{\vec{\sigma}\cdot\vec{r}_v}{m}\right] \tag{A.17}$$

$$+ \frac{1}{2}\frac{d\ \ell n\ s}{dx} + \frac{\kappa\zeta - s}{\zeta - \kappa s}\frac{\vec{\sigma}\cdot\vec{r}}{2\eta^2 u}\left[\kappa(2-\eta) + \frac{(2-3\eta)\zeta}{s}\right]$$

is singular at a Class II turning point, where $(\zeta - \kappa s)$ vanishes. It is seen from Eq. (3.7) that the first correction term to $\vec{\theta}_1$ is singular, then, even though the leading term is regular.

APPENDIX B

In this appendix, we prove that unstable roots of $V(\tau, \epsilon)$ occur in conjugate pairs in the τ-plane. For this purpose, it is sufficient to show that, by suitable choice of the arbitrary multiplicative constant in $\vec{\theta}(x, \tau, \epsilon)$, $V(\tau, \epsilon)$ is an analytic function of τ and is real for all real values of τ.

Now V is given by Eq. (2.3) which can be written in the following fashion, using the vectors $\vec{g}_t$, $\vec{g}_y$, $\vec{h}_t$, and $\vec{h}_y$ of Ref. 3:

$$V(\tau, \epsilon) = \int_0^\infty \vec{\theta} \cdot \underset{\sim}{A}^{-1} \cdot \left\{ \tau \begin{bmatrix} g_{t1} \\ g_{t2} \\ 0 \\ g_{t4} \\ g_{t5} \end{bmatrix} + i\epsilon \begin{bmatrix} 0 \\ 0 \\ g_{y3} \\ 0 \\ 0 \end{bmatrix} \right\} dx$$

$$- \vec{\theta}(0, \tau, \epsilon) \cdot \left\{ \tau \begin{bmatrix} h_{t1} \\ h_{t2} \\ 0 \\ h_{t4} \\ h_{t5} \end{bmatrix} + i\epsilon \begin{bmatrix} 0 \\ 0 \\ h_{y3} \\ 0 \\ 0 \end{bmatrix} \right\} \qquad \text{(B.1)}$$

From Appendix A, Eq. (A.1), it is seen that the products of $\underset{\sim}{A}^{-1}$ with the $\vec{g}$ vectors have the same zero elements as the $\vec{g}$'s themselves. It follows, then, that $V(\tau, \epsilon)$ is real and analytic (for real τ) if $\vec{\theta}$ is analytic and

$$\mathrm{Re}[\vec{\theta}(x, \tau, \epsilon)] \cdot \hat{e}_3 = 0$$

$$\mathrm{Im}[\vec{\theta}(x, \tau, \epsilon)] \cdot \hat{e}_i = 0, \qquad i = 1, 2, 4, 5. \tag{B.2}$$

Now the differential equation for $\vec{\theta}$, Eq. (2.4), has the coefficient matrix $-\underset{\sim}{P}'(x, \tau, \epsilon)$

$$-\underset{\sim}{P}'(x, \tau, \epsilon) = \{\underset{\sim}{A}_x^{-1} \cdot [\tau \underset{\sim}{I} + i\epsilon \underset{\sim}{A}_y + \underset{\sim}{B}]\}' \tag{B.3}$$

which has real part

$$\{\underset{\sim}{A}_x^{-1} \cdot [\tau \underset{\sim}{I} + \underset{\sim}{B}]\}' \tag{B.4}$$

and imaginary part

$$\epsilon(\underset{\sim}{A}_x^{-1} \cdot \underset{\sim}{A}_y)' \, . \tag{B.5}$$

From the fact that $\underset{\sim}{B}$ has only zero elements in column 3 and in row 3 [See Appendix A, Eq. (A.11), (A.12)], it follows that the real part of $-\underset{\sim}{P}'$ is diagonal with respect to element 3, i.e., it has the same block diagonal form of $\underset{\sim}{A}_x^{-1}$,

$$\begin{bmatrix} M_{11} & M_{12} & 0 & M_{14} & M_{15} \\ M_{21} & M_{22} & 0 & M_{24} & M_{25} \\ 0 & 0 & M_{33} & 0 & 0 \\ M_{41} & M_{42} & 0 & M_{44} & M_{45} \\ M_{51} & M_{52} & 0 & M_{54} & M_{55} \end{bmatrix} \tag{B.6}$$

On the other hand, the imaginary part is found to be of just the

complementary form, i.e., it has non-zero elements only in the off-diagonal positions of row 3 and column 3. Hence, if $\vec{\theta}$ has the form of Eq. (B.2), then $d\vec{\theta}/dx$ also does, and, by repeated differentiation, so do all its derivatives. If, therefore, $\vec{\theta}$ has the form of Eq. (B.2) for any x_o, it does so for all x.

Unfortunately the only point in the reaction zone where $\vec{\theta}$ can be determined is in the equilibrium state, $x \to \infty$. It turns out, however, that the property (B.2) holds in this limit and its validity there is sufficient to establish it everywhere. We begin by demonstrating that the asymptotic form[3] of $\vec{\theta}$, as $x \to \infty$,

$$\vec{\theta}(x, \tau, \epsilon) \sim e^{x\mu(\tau, \epsilon)} \vec{\nu}(\tau, \epsilon) \tag{B.7}$$

has the property (B.2). Now $\mu(\tau,\epsilon)$ is the eigenvalue of $-\underset{\sim}{P}'(\infty,\tau, \epsilon)$ having negative real part and $\vec{\nu}(\tau, \epsilon)$ is the associated eigenvector. Since $\underset{\sim}{P}$ is analytic in τ, μ is also analytic and $\vec{\nu}$ can be chosen to be analytic.[26] Now the complex conjugate of $-\underset{\sim}{P}'$ has a single eigenvalue with negative real part. It can be seen from the properties previously ascribed to its real and imaginary parts, Eq. (B.4) and (B. 5), that the following relationship holds:

$$-\underset{\sim}{P}'^{*}(\infty, \tau, \epsilon) \cdot \vec{\nu}_1(\tau, \epsilon) = \mu(\tau, \epsilon)\vec{\nu}_1(\tau, \epsilon)$$

$$\vec{\nu}_1(\tau, \epsilon) = \begin{bmatrix} \nu_1 \\ \nu_2 \\ -\nu_3 \\ \nu_4 \\ \nu_5 \end{bmatrix} \tag{B.8}$$

where * denotes the complex conjugate. Thus

$$\mu^*(\tau, \epsilon) = \mu(\tau, \epsilon) \tag{B.9}$$

and μ is real. Moreover, $\vec{\nu}_1^*$ is also an eigenvector of $-\underset{\sim}{P}'$, whence the eigenvector

$$\vec{\nu}_2(\tau, \epsilon) = \tfrac{1}{2}[\vec{\nu} + \vec{\nu}_1^* - i(\vec{\nu} - \vec{\nu}_1^*)] \tag{B.10}$$

has the property (B.2).

To complete the proof, we obtain an explicit solution for $\vec{\theta}$, valid in the neighborhood of equilibrium. To do this, define a new independent variable

$$\bar{z}(x) = \left[\frac{S(\infty) - S(x)}{S(\infty) - S(0)}\right]^{\frac{1}{2}} \tag{B.11}$$

where $S(x)$ is the entropy in the steady reaction zone which is constrained to increase monotonically with x by virtue of the second law of thermodynamics.[7] Thus $\bar{z}(x)$ varies monotonically between 1 at the shock and 0 at $x = \infty$.

The differential equation for $\vec{\theta}$ becomes

$$\frac{d\vec{\theta}}{d\bar{z}} = \underset{\sim}{\Omega}(\bar{z}, \tau, \epsilon) \cdot \vec{\theta}$$

$$\underset{\sim}{\Omega} = \frac{2\bar{z}u}{\hat{\Phi}} \underset{\sim}{P}'(x, \tau, \epsilon) \tag{B.12}$$

where $\hat{\Phi}$ is the entropy production, $-\vec{\Delta F}\cdot\vec{r}/T$, a non-negative thermodynamic function. The $\bar{z} = 0$ point is a singular point of $\underset{\sim}{\Omega}$ by virtue of the fact the $\hat{\Phi}$ vanishes.

Now throughout the reaction zone, the thermodynamic functions of state, under the steady-state constraints, were shown by Wood and Salsburg[7] to be regular functions of the progress variables $\vec{\lambda}$, so that $\underset{\sim}{P}$ itself is regular at $\bar{z} = 0$. Near equilibrium, the entropy production Φ is of second order in $\vec{\lambda} - \vec{\lambda}(\infty)$, and the entropy gradient in $\vec{\lambda}$-space is of first order. Thus $\vec{\lambda} - \vec{\lambda}(\infty)$ vanishes linearly in $\bar{z}$, and $\underset{\sim}{\Omega}$ has a simple pole at $\bar{z} = 0$. In some neighborhood of $\bar{z} = 0$, the series

$$\underset{\sim}{\Omega} = (\bar{z})^{-1} \sum_{k=0}^{\infty} \bar{z}^k \underset{\sim}{\Omega}_k \tag{B.13}$$

converges, and the leading term $\underset{\sim}{\Omega}_0$ is proportional to $\underset{\sim}{P}'(\infty, \tau, \epsilon)$. Convergent power series solutions of Eq. (B.12) can be derived by application of the theory of singularities of the first kind[27], and the lone solution bounded at $\bar{z} = 0$ can be picked out, viz.

$$\vec{\theta}(\bar{z}, \tau, \epsilon) = \bar{z}^{\tilde{\mu}} \left[\underset{\sim}{I} + \bar{z} \sum_{k=0}^{\infty} \underset{\sim}{G}_k \bar{z}^k \right] \cdot \vec{\nu}_2 \ . \tag{B.14}$$

Here we have employed $\tilde{\mu}$ and $\vec{\nu}_2$ for the eigenvalue and eigenvector of $\underset{\sim}{\Omega}_0$, so that $\tilde{\mu}$ is real and positive [opposite in sign to μ of Eq. (B.7)] and $\vec{\nu}_2$ is given by Eq. (B.10) to have property (B.2). Now by Eq. (B.14) the quantity

$$\vec{\bar{\theta}} = (\bar{z})^{-\tilde{\mu}} \vec{\theta}(\bar{z}, \tau, \epsilon) \tag{B.15}$$

is regular at $\bar{z} = 0$, and its derivative

$$\left(\underset{\sim}{\Omega} - \frac{\tilde{\mu}}{\bar{z}} \underset{\sim}{I} \right) \cdot \vec{\bar{\theta}} = \left[\frac{2\bar{z}u}{\Phi} \underset{\sim}{P}' - \frac{\tilde{\mu}}{\bar{z}} \underset{\sim}{I} \right] \vec{\bar{\theta}} \tag{B.16}$$

will also have the property (B.2) at this point, as follows from the previously discussed properties of $\underset{\sim}{P}'$. In fact, all the derivatives obviously do; and, since these are precisely the higher coefficients in Eq. (B.14), it follows that $\vec{\theta}$ itself has the desired property.

APPENDIX C

The transformations of Sec. 6 begin with $\underset{\sim}{Q}_0$ which satisfies Eq. (6.6)

$$[\underset{\sim}{\Phi}_0 - \tfrac{1}{2}(\mu_1 + \mu_2)\underset{\sim}{I}] \cdot \underset{\sim}{Q}_0 = \underset{\sim}{Q}_0 \cdot \underset{\sim}{L}_0 \cdot \tag{C.1}$$

The simplest route to finding $\underset{\sim}{Q}_0$ is by first diagonalizing the coefficient matrix on the left. We have, from Appendix A,

$$\underset{\sim}{T}^{-1} \cdot [\underset{\sim}{\Phi}_0 - \tfrac{1}{2}(\mu_1 + \mu_2)\underset{\sim}{I}] \cdot \underset{\sim}{T} = \text{Diag}\,[-\mu_{21}/2,\ \mu_{21}/2,\ n(x),\ \ldots,\ n(x)] \tag{C.2}$$

and we require the transform

$$\text{Diag}\,[-\mu_{21}/2,\ \ldots,\ n(x)] \cdot \underset{\sim}{\Xi} = \underset{\sim}{\Xi} \cdot \underset{\sim}{L}_0. \tag{C.3}$$

One readily finds

$$\underset{\sim}{\Xi} = \begin{bmatrix} -\frac{1}{2} & \eta u/2\kappa s & 0 \\ -\frac{1}{2} & -\eta u/2\kappa s & \\ 0 & & \underset{\sim}{I}_{n+2} \end{bmatrix} \tag{C.4}$$

Thus

$$\underset{\sim}{Q}_0 = \underset{\sim}{T} \cdot \underset{\sim}{\Xi} \tag{C.5}$$

has columns

$$\underset{\sim}{Q}_0 \cdot \hat{e}_1 = \begin{bmatrix} 0 \\ -\zeta/u \\ i \\ 0 \\ 0 \end{bmatrix}, \qquad \underset{\sim}{Q}_0 \cdot \hat{e}_2 = \begin{bmatrix} m\eta/(1-\eta) \\ 0 \\ 0 \\ -\eta p_S/m \\ -\eta \vec{p}_\lambda/m \end{bmatrix}$$

$$\underset{\sim}{Q}_0 \cdot \hat{e}_j = \underset{\sim}{T} \cdot \hat{e}_j, \qquad j = 3,\ 4,\ \ldots,\ n+4. \tag{C.6}$$

Moreover, since we had

$$\underset{\sim}{E} = \underset{\sim}{T}^{-1} \cdot [\underset{\sim}{\Phi}_1 \cdot \underset{\sim}{T} - d\underset{\sim}{T}/dx]$$

we have for the matrix $\underset{\sim}{H}$, Eq. (6.6)

$$\underset{\sim}{H} = \underset{\sim}{\Xi}^{-1} \cdot [\underset{\sim}{E} \cdot \underset{\sim}{\Xi} - d\underset{\sim}{\Xi}/dx] \,. \tag{C.7}$$

Thus $\underset{\sim}{H}$ differs from $\underset{\sim}{E}$ only in the first two columns,

$$\underset{\sim}{H} \cdot \hat{e}_1 = \begin{bmatrix} \frac{1}{2}(E_{11} + E_{12} + E_{21} + E_{22}) \\ -\frac{\kappa s}{2\eta u}(E_{11} + E_{12} - E_{21} - E_{22}) \\ -\frac{1}{2}(E_{31} + E_{32}) \\ -\frac{1}{2}(E_{41} + E_{42}) \\ -\frac{1}{2}(E_{51} + E_{52}) \end{bmatrix}$$

$$\underset{\sim}{H} \cdot \hat{e}_2 = \begin{bmatrix} -\frac{\eta u}{2\kappa s}(E_{11} - E_{12} + E_{21} - E_{22}) \\ \frac{1}{2}(E_{11} - E_{12} - E_{21} + E_{22}) - d\,\ell n(\eta u/\kappa s)/dx \\ \frac{\eta u}{2\kappa s}(E_{31} - E_{32}) \\ \frac{\eta u}{2\kappa s}(E_{41} - E_{42}) \\ \frac{\eta u}{2\kappa s}(E_{51} - E_{52}). \end{bmatrix} \tag{C.8}$$

It should be emphasized that, despite the appearance of $\underset{\sim}{E}$ and s in Eq. (C.7) and (C.8), $\underset{\sim}{H}$ is a regular function of x by virtue of Eq. (6.6), (C.6), and (A.6).

In order to prove the existence of the transforms Eq. (6.10), we employ induction. Thus we first show that the transformation

$$\vec{\Psi}_{(0)} = \underset{\sim}{S}_1 \cdot \vec{\Psi}_{(1)}$$

$$\underset{\sim}{S}_1 = [\underset{\sim}{I} + \epsilon^{-1}\underset{\sim}{Q}_1] \exp \int_0^x g_0 dx' \tag{C.9}$$

yields

$$\frac{d\vec{\Psi}_{(1)}}{dx} = [\epsilon \underset{\sim}{L}_0(x) + \underset{\sim}{L}_1(x) + \epsilon^{-1}\underset{\sim}{U}^{(1)}(x, \epsilon)] \cdot \vec{\Psi}_{(1)} \cdot \tag{C.10}$$

Now differentiation of Eq. (C.9) yields

$$\frac{d\vec{\Psi}_{(1)}}{dx} = \epsilon \underset{\sim}{\Lambda}_1 \cdot \vec{\Psi}_{(1)} \tag{C.11}$$

$$\epsilon \underset{\sim}{\Lambda}_1 = (\underset{\sim}{I} + \epsilon^{-1}\underset{\sim}{Q}_1)^{-1} \cdot [(\epsilon \underset{\sim}{L}_0 + \underset{\sim}{H}) \cdot (\underset{\sim}{I} + \epsilon^{-1}\underset{\sim}{Q}_1) - \epsilon^{-1} d\underset{\sim}{Q}_1/dx] - g_0 \underset{\sim}{I}.$$

Using the identity

$$(\underset{\sim}{I} + \epsilon^{-1}\underset{\sim}{Q}_1)^{-1} = \underset{\sim}{I} - \epsilon^{-1}\underset{\sim}{Q}_1 + \epsilon^{-2}\underset{\sim}{Q}_1^2 \cdot (\underset{\sim}{I} + \epsilon^{-1}\underset{\sim}{Q}_1)^{-1} ,$$

we have

$$\begin{aligned} \epsilon \underset{\sim}{\Lambda}_1 = {} & \epsilon \underset{\sim}{L}_0 + (\underset{\sim}{L}_0 \cdot \underset{\sim}{Q}_1 - \underset{\sim}{Q}_1 \cdot \underset{\sim}{L}_0 + \underset{\sim}{H} - g_0 \underset{\sim}{I}) \\ & + \epsilon^{-1}[\underset{\sim}{Q}_1^2 \cdot (\underset{\sim}{I} + \epsilon^{-1}\underset{\sim}{Q}_1)^{-1} \cdot \underset{\sim}{L}_0 - \underset{\sim}{Q}_1 \cdot (\underset{\sim}{I} + \epsilon^{-1}\underset{\sim}{Q}_1)^{-1} \cdot (\underset{\sim}{H} + \underset{\sim}{L}_0 \cdot \underset{\sim}{Q}_1) \\ & + (\underset{\sim}{I} + \epsilon^{-1}\underset{\sim}{Q}_1)^{-1} \cdot (\underset{\sim}{H} \cdot \underset{\sim}{Q}_1 - d\underset{\sim}{Q}_1/dx)] . \end{aligned} \tag{C.12}$$

The terms within the bracket have the desired power series expansion irrespective of the choice of $\underset{\sim}{Q}_1$ and g_0 so that we need only show that

$$\underset{\sim}{L}_0 \cdot \underset{\sim}{Q}_1 - \underset{\sim}{Q}_1 \cdot \underset{\sim}{L}_0 + \underset{\sim}{H} - g_0 \underset{\sim}{I} = \underset{\sim}{L}_1 \tag{C.13}$$

for suitable choices for $\underset{\sim}{Q}_1$ and g_0.

To solve Eq. (C.13), it is convenient to drop the subscripts on $\underset{\sim}{Q}_1$ and write the matrices in block form,

$$\underset{\sim}{H} = \begin{bmatrix} \underset{\sim}{H}_{11} & \underset{\sim}{H}_{12} \\ \underset{\sim}{H}_{21} & \underset{\sim}{H}_{22} \end{bmatrix} , \quad \underset{\sim}{L}_0 = \begin{bmatrix} \underset{\sim}{L}^{\circ}_{11} & 0 \\ 0 & \underset{\sim}{L}^{\circ}_{22} \end{bmatrix}$$

where $\underset{\sim}{H}_{11}$ is a 2-by-2 matrix and $\underset{\sim}{H}_{22}$ is an $(n + 2)$-by-$(n + 2)$. Then Eq. (C.13) becomes

$$\underset{\sim}{H}_{11} - g_0\underset{\sim}{I}_2 - \underset{\sim}{Q}_{11} \cdot \underset{\sim}{L}^{\circ}_{11} + \underset{\sim}{L}^{\circ}_{11} \cdot \underset{\sim}{Q}_{11} = \underset{\sim}{L}^{1}_{11} \tag{C.14a}$$

$$\underset{\sim}{H}_{12} - \underset{\sim}{Q}_{12} \cdot \underset{\sim}{L}^{\circ}_{22} + \underset{\sim}{L}^{\circ}_{11} \cdot \underset{\sim}{Q}_{12} = 0 \tag{C.14b}$$

$$\underset{\sim}{H}_{21} - \underset{\sim}{Q}_{21} \cdot \underset{\sim}{L}^{\circ}_{11} + \underset{\sim}{L}^{\circ}_{22} \cdot \underset{\sim}{Q}_{21} = 0 \tag{C.14c}$$

$$\underset{\sim}{H}_{22} - g_0\underset{\sim}{I}_{n+2} - \underset{\sim}{Q}_{22} \cdot \underset{\sim}{L}^{\circ}_{22} + \underset{\sim}{L}^{\circ}_{22} \cdot \underset{\sim}{Q}_{22} = \underset{\sim}{L}^{1}_{22} . \tag{C.14d}$$

Since $\underset{\sim}{L}^{\circ}_{22}$ is $n(x)\underset{\sim}{I}_{n+2}$, Eq. (6.7), we have

$$\underset{\sim}{Q}_{12} \cdot \underset{\sim}{L}^{\circ}_{22} = n(x)\underset{\sim}{Q}_{12},$$

whence Eq. (C.14b) yields

$$\underset{\sim}{Q}_{12} = - [\underset{\sim}{L}^{\circ}_{11} - n(x)\underset{\sim}{I}_2]^{-1} \cdot \underset{\sim}{H}_{12} . \tag{C.15}$$

The inverse matrix on the right exists by virtue of the fact that the eigenvalues of $\underset{\sim}{L}^{\circ}_{11}$ are distinct from $n(x)$. Similarly, Eq. (C.14c) has solution

$$\underset{\sim}{Q}_{21} = \underset{\sim}{H}_{21} \cdot [\underset{\sim}{L}^{o}_{11} - n(x)\underset{\sim}{I}_{2}]^{-1} \cdot \qquad \text{(C.16)}$$

In view of the character of $\underset{\sim}{L}^{o}_{22}$, it is also evident that $\underset{\sim}{Q}_{22}$ disappears from Eq. (C.14d) and, thus, does not appear in Eq. (C.14) at all. Hence, we can simply write

$$\underset{\sim}{Q}_{22} = 0$$

$$\underset{\sim}{L}^{1}_{22} = \underset{\sim}{H}_{22} - g_{0}\underset{\sim}{I}_{n+2}. \qquad \text{(C.17)}$$

Finally, Eq. (C.14a) becomes in component notation (i.e., dropping subscripts from $\underset{\sim}{Q}_{11}$ and $\underset{\sim}{H}_{11}$, but inserting subscripts for the four individual elements),

$$H_{11} - g_{0} + \ell_{0}Q_{12} + Q_{21} = 0 \qquad \text{(C.18a)}$$

$$H_{12} - Q_{11} + Q_{22} = 0 \qquad \text{(C.18b)}$$

$$H_{21} + \ell_{0}Q_{22} - \ell_{0}Q_{11} = -\ell_{1} \qquad \text{(C.18c)}$$

$$H_{22} - g_{0} - Q_{21} - \ell_{0}Q_{12} = 0. \qquad \text{(C.18d)}$$

Combining Eq. (C.18b) and (C.18c), we readily obtain

$$\ell_{1} = \ell_{0}H_{12} - H_{21}$$

$$Q_{11} - Q_{22} = H_{12} \cdot \qquad \text{(C.19)}$$

Adding Eq. (C.18a) and (C.18d), we get

$$g_{0} = \tfrac{1}{2}(H_{11} + H_{22}) \qquad \text{(C.20)}$$

which serves to determine g_{0}. The proof is completed by choosing

$$Q_{12} = 1$$

$$Q_{21} = - \ell_0 + \tfrac{1}{2} (H_{22} - H_{11}) \qquad \text{(C.21)}$$

$$Q_{11} = H_{12}$$

$$Q_{22} = 0 \, .$$

To complete the inductive proof of Eq. (6.10), we assume its validity for k - 1, with $k \geq 2$, and examine the next transformation

$$\vec{\Psi}_{(k-1)} = \underset{\sim}{S}_k \cdot \vec{\Psi}_{(k)}$$

$$\frac{d\vec{\Psi}_{(k)}}{dx} = \epsilon \underset{\sim}{\Lambda}_k \cdot \vec{\Psi}_{(k)} \qquad \text{(C.22)}$$

$$\epsilon \underset{\sim}{\Lambda}_k = (\underset{\sim}{I} + \epsilon^{-k} \underset{\sim}{Q}_k)^{-1} \cdot [\epsilon \underset{\sim}{\Lambda}_{k-1} \cdot (\underset{\sim}{I} + \epsilon^{-k} \underset{\sim}{Q}_k)$$

$$- \epsilon^{-k} d\underset{\sim}{Q}_k/dx] - \epsilon^{-k+1} g_{k-1} \underset{\sim}{I} \, .$$

Employing the identity

$$(\underset{\sim}{I} + \epsilon^{-k} \underset{\sim}{Q}_k)^{-1} = \underset{\sim}{I} - \epsilon^{-k} \underset{\sim}{Q}_k + \epsilon^{-2k} \underset{\sim}{Q}_k^2 \cdot (\underset{\sim}{I} + \epsilon^{-k} \underset{\sim}{Q}_k)^{-1} \, ,$$

we have, from the properties of $\underset{\sim}{\Lambda}_{k-1}$, Eq. (6.10),

$$\epsilon \underset{\sim}{\Lambda}_k = \epsilon \underset{\sim}{L}^{(k-1)} + \epsilon^{-k+1} (\underset{\sim}{U}_0^{(k-1)} - \underset{\sim}{Q}_k \cdot \underset{\sim}{L}_0 + \underset{\sim}{L}_0 \cdot \underset{\sim}{Q}_k - g_{k-1} \underset{\sim}{I}) \qquad \text{(C.23)}$$

$$+ \epsilon^{-k} \{ \cdots\cdots \} .$$

We do not write out the terms in the bracket, but it is evident from Eq. (C.22) that this remainder has a power series expansion. The coefficient of ϵ^{-k+1}, on the other hand, agrees with that for k = 1,

Eq. (C.12), except in the subscripts on the unknowns and the symbol for the "knowns" $\underset{\sim}{H}$ and $\underset{\sim}{U}_0^{(k-1)}$, whence

$$\underset{\sim}{U}_0^{k-1} - \underset{\sim}{Q}_k \cdot \underset{\sim}{L}_0 + \underset{\sim}{L}_0 \cdot \underset{\sim}{Q}_k - g_{k-1}\underset{\sim}{I} = \underset{\sim}{L}_k \qquad (C.24)$$

has a solution of precisely the same form as before. The proof is therefore complete.

APPENDIX D

The proof of the asymptotic equivalence of the (transformed) given differential Eq. (6.11) and the (transformed) related Eq. (6.12), i.e., the proof of Eq. (6.43), is briefly outlined here. It depends upon consideration of the integral equation for the solutions of Eq. (6.11),

$$\vec{\psi}_\nu(x, \epsilon) = \vec{y}_\nu(x, \epsilon) + \epsilon^{-m} \underset{\sim}{Y}(x, \epsilon) \cdot \int^x \underset{\sim}{Y}^{-1}(s, \epsilon) \cdot \underset{\sim}{\Gamma}(s, \epsilon) \cdot \vec{\psi}_\nu(s, \epsilon) ds$$

$$\underset{\sim}{\Gamma}(x, \epsilon) = \underset{\sim}{U}(x, \epsilon) - \underset{\sim}{J}(x, \epsilon) \qquad \text{(D.1)}$$

where $\underset{\sim}{Y}$ denotes the matrix of columns $\vec{y}_i$, Eq. (6.42), and where the lower limit of the integral on the right may depend upon the "matrix element" within the integral; i.e., if the integrand is written as a sum, the lower limit may vary from term to term. The validity of Eq. (D.1) is readily established by differentiation.

In order to establish Eq. (6.43), it is conducive to clarity to consider the specific case $\delta = i$ in Eq. (6.26), corresponding to a turning point x^* at which $c_o^2 \eta$ is a maximum. In fact, we will simply restrict our attention to profile M, Fig. 5, for which there are no other turning points on the x axis. By virtue of this specification, the "stretched" variable ψ, Eq. (6.28) has argument $\pi/2$ for $z > 0$ and $5\pi/2$ for $z < 0$. Turning to the asymptotic expressions Eq. (6.40) and (6.41), we find that the behavior of these functions with increasing ϵ (i.e., increasing $|\omega|$) depends on the $\psi^{\pm k - \frac{1}{4}}$ terms rather than on the exponentials in ψ.

To prove the desired asymptotic result, it is important that the set of n + 4 known solutions of the related equation, $\vec{y}_i (i = 1, \ldots, n + 4)$, be "asymptotically distinguishable" for all x. This property is illustrated by the solutions $\vec{y}_1$ and $\vec{y}_2$ if we assume that Re(k) < 0. From Eq. (6.40) and (6.41), it follows that $\vec{y}_1 = \vec{y}^{(0)}$ is recessive relative to $\vec{y}_2 = \vec{y}^{(2)}$ for z > 0, while for z < 0, $\vec{y}^{(2)}$ is recessive. By virtue of the fact that one is recessive while one is dominant for all z, these are said to be asymptotically distinguishable.

For the case of Re(k) > 0, $\vec{y}^{(0)}$ and $\vec{y}^{(2)}$ remain linearly independent solutions. However, the leading part (for large ϵ) of each is of the dominant type, as is seen from Eq. (6.40) and (6.41). Therefore, asymptotically they are not distinguishable and are not suitable in the proof of Eq. (6.43). In this instance, it can be demonstrated that the pair $\vec{y}^{(1)}$ and $\vec{y}^{(3)}$ given through Eq. (6.39) are distinguishable and should be used for $\vec{y}_1$ and $\vec{y}_2$ in the proof, i.e., in place of Eq. (6.42).

For $\vec{y}_1$ and $\vec{y}_2$ in the case Re(k) = 0 and for the solutions of the (n + 2)-order related equation, $\vec{y}_3, \ldots, \vec{y}_{n+4}$, the concept of asymptotic distinguishability is not particularly important; for the various solutions do not become recessive or dominant for large ϵ. Instead, the leading parts of these solutions in the $\epsilon \to \infty$ limit remain linearly independent.

In view of the distinguishability of $\vec{y}_1$ and $\vec{y}_2$ as defined in Eq. (6.42) for Re(k) < 0, we will restrict our attention to this case in the remainder of this Appendix. The Re(k) > 0 case is equivalent, once

$\vec{y}_1$ and $\vec{y}_2$ have been redefined in the manner indicated above.

The proof is based upon an adaptation of the theorem used by Langer:[9] Given the integral equation

$$\vec{f}(x, \epsilon) = \vec{g}(x, \epsilon) + \epsilon^{-m} \int^{x} \underset{\sim}{K}(x, s, \epsilon) \cdot \vec{f}(s, \epsilon) ds \qquad \text{(D.2a)}$$

with the order relations

$$\vec{g}(x, \epsilon) = h(x, \epsilon) O(1)$$

$$\int^{x} \underset{\sim}{K}(x, s, \epsilon) \frac{h(s,\epsilon)}{h(x,\epsilon)} ds = O(1), \qquad \epsilon \to \infty , \qquad \text{(D.2b)}$$

then

$$\vec{f}(x, \epsilon) = \vec{g}(x, \epsilon) + h(x, \epsilon) O(\epsilon^{-m}). \qquad \text{(D.2c)}$$

The norm to be used for the arrays is the maximum absolute value of the elements. The proof of the theorem is essentially given by Langer.

To begin with, then, we require the kernel of our integral equation in somewhat greater detail. In particular, the inverse of $\underset{\sim}{Y}$ is required. From Eq. (6.17), (6.24), (6.39), and (6.42) we obtain

$$\underset{\sim}{Y}^{-1} = \begin{bmatrix} \frac{1}{F(\epsilon)} \begin{bmatrix} \epsilon^{-1} u_2' & -u_2 \\ \epsilon^{-1} u_0' & u_0 \end{bmatrix} & 0 \\ 0 & \underset{\sim}{C}^{-1}(x, \epsilon) \exp \int_0^x -\epsilon n(x') dx' \end{bmatrix} \qquad \text{(D.3)}$$

where F is the determinant of the upper 2-by-2 part of $\underset{\sim}{Y}$ and hence is ϵ^{-1} times the Wronskian of the solutions u_0 and u_2 of Eq. (6.27). By virtue

of the absence of a first derivative term in the latter, F is independent of x and is found, following McKelvey,[10] to be proportional to $\epsilon^{-\frac{1}{2}}$. Since n(x), Eq. (6.7), is pure imaginary and $\underset{\sim}{C}$ is a polynomial in ϵ^{-1}, the (n + 2)-by-(n + 2) block of $\underset{\sim}{Y}^{-1}$ is a bounded function of ϵ. Since $\underset{\sim}{\Gamma}(x, \epsilon)$, Eq. (D.1), has a power series expansion at $1/\epsilon = 0$, it is bounded in ϵ and the behavior of each element of the kernel of the differential equation is known.

One now can apply the theorem (D.2) on any finite x interval, say (0, 2x*), which includes the turning point. Since the behavior of the $\vec{y}_1$ and $\vec{y}_2$ columns of $\underset{\sim}{Y}$ depends critically on the value of x, we divide this interval into three subintervals (0, x_-), (x_-, x_+), and (x_+, 2x*) by the condition

$$|\psi[z(x_\pm), i\epsilon]| = M \tag{D.4}$$

with M some large positive number. Since ψ is linear in ϵ and of order $(x - x^*)^2$ near the turning point, the central subinterval, containing the point x*, has length of order $\epsilon^{-\frac{1}{2}}$.

By virtue of this decomposition, we can apply the $z > 0$ asymptotic formulas for $\vec{y}_1$ and $\vec{y}_2$, Eq. (6.40a) and (6.41a), on the interval (x_+, 2x*), and the $z < 0$ formulas Eq. (6.40b) and (6.41b) on (0, x_-). On the central subinterval, however, the asymptotic formulas no longer apply so that we return to the full expression for the $u_\nu(z, \hat{\omega})$ functions in Eq. (6.29). Since ψ is bounded, it follows from the power series Eq. (6.31) that the $v_\nu(z, \hat{\omega})$ functions in Eq. (6.29e) are also bounded.

In addition, it can be shown from this power series that, although the derivatives of the confluent hypergeometric functions are infinite at $\psi = 0$ (i.e., at the turning point), it is nonetheless true that v_ν' and v_ν'' are bounded throughout the subinterval (x_-, x_+). Thus u_ν and its derivative, which determine y_1 and y_2 through Eq. (6.39), are also bounded.

To prove admissibility of either $\vec{y}_1$ or $\vec{y}_2$, we begin on the subinterval on which it is recessive, setting the lower integration limit, for all matrix elements, in Eq. (D.1) to the outer limit of the interval, i.e., either 0 or $2x^*$. For the sake of illustration, we will consider the admissibility of $\vec{y}_1$, so that we begin on $(x_+, 2x^*)$. We set the function $h(x, \epsilon)$ of the theorem to $\psi^{k-\frac{1}{4}}$, so that, by Eq. (6.40a), the order relation for the inhomogeneous part in Eq. (D.2) holds. The required order relation for the kernel can then be established through the asymptotic expressions for $\vec{y}_1$ and $\vec{y}_2$ and the boundedness of $\vec{y}_3$, $\vec{y}_4$, ..., thereby proving admissibility on one subinterval.

On the central interval, the function $h(x, \epsilon)$ in the theorem becomes simply unity, and the integral is split into a contribution over the outer subinterval $(x_+, 2x^*)$ and one from x_+ to x. The first contribution involves only known functions, since $\vec{\psi}_1$ on $(x_+, 2x^*)$ was just found to be $\vec{y}_1$ in the last paragraph, and is grouped with the inhomogeneous part of Eq. (D.1) to form the inhomogeneous part $\vec{g}(x, \epsilon)$ of the theorem. The order relations are once more established using the boundedness of the $\vec{y}_i$ within the (x_-, x_+) and the fact that the

interval of integration is of order $\epsilon^{-\frac{1}{2}}$. Thus $\vec{\psi}_1$ is proved equal to $\vec{y}_1$, to order ϵ^{-m}, on $(x_-, 2x^*)$.

The final interval $(0, x_-)$ is considered by combining the integral from x_- to $2x^*$ in Eq. (D.1) with $\vec{y}_1$ to form $\vec{g}(x, \epsilon)$ for Eq. (D.2). One shows that this part satisfies the first of Eq. (D.2b) for $h = \psi^{-k-\frac{1}{4}}$ and then turns to the inhomogeneous part, using again the known asymptotic expressions. The proof of admissibility is then complete.

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20. See Ref. 10 and Ref. 17, pp. 342-345.

21. Ref. 17, example 3, p. 352.

22. Ref. 17, p. 338.

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