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State of Detonation Stability Theory and Its Application to Propulsion

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We present an overview of the current state of detonation stability theory and discuss its implications for propulsion. The emphasis of the review is on the exact or asymptotic treatments of detonations, including various asymptotic limits that appear in the literature. The role that instability plays in practical detonation-based propulsion is of primary importance and is largely unexplored, hence we point to possible areas of research both theoretical and numerical, that might help improve our understanding of detonation behavior in propulsion devices. We outline the basic formulation of detonation stability theory that starts from linearized Euler equations, describe the algorithm of solution, and present an example that illustrates typical results.

Nomenclature

c = sound speed
D = one-dimensional detonation speed
$\boldsymbol{D}$ = shock velocity vector
E = activation energy
e = internal energy per unit mass including chemical energy
f = degree of overdrive
$\mathcal{H}$ = enthalpy flux across the shock
k = transverse wave number
k_ω = reaction rate constant
M = local Mach number relative to the shock
$\mathcal{M}$ = mass flux across the shock
n = shock-attached frame axial coordinate
$\boldsymbol{n}$ = unit normal to the shock
$\mathcal{P}$ = momentum flux across the shock
p = pressure
Q = heat release per unit mass
$\boldsymbol{q}$ = state vector
$\boldsymbol{t}$ = unit tangent vector to the shock
U = x component of particle velocity in steady shock frame
U_1 = x component of particle velocity in unsteady shock frame
$\boldsymbol{u}$ = particle velocity vector in laboratory frame
u_1 = x component of particle velocity in laboratory frame
u_2 = y component of particle velocity
v = specific volume
x = laboratory frame axial coordinate
y = transverse coordinate
α = perturbation growth rate
γ = ratio of specific heats
λ = reaction progress variable
ρ = density
σ = thermicity
ψ = shock displacement from the steady position along x axis
ω = reaction rate

Subscript

CJ = Chapman–Jouguet
i = variable number
n = normal to the shock

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p	=	partial derivative with respect to p
s	=	the shock state
v	=	partial derivative with respect to v
λ	=	partial derivative with respect to λ
0	=	ambient state
1	=	along x axis
2	=	along y axis
∞	=	evaluated at ∞

Superscript

*	=	steady base state
′	=	perturbation

I. Introduction

THE plan of this article is to give a focused review that defines the current state of detonation stability theory and to highlight the most well-established and informative results that could be used to understand detonative processes, some with application to propulsion. The charge given to us by the editors was partly to define the importance of detonation stability to propulsion, and in this matter we rely in part on some of the excellent work and reviews on propulsion scenarios that use (or potentially use) detonation [1–4] (some of which have appeared in this journal). These scenarios principally include ramjets, scramjets, oblique detonation wave, and pulsed detonation engines. All, except for pulsed detonation, propose to stabilize a detonation in a premixed, detonable fuel/oxidant stream, and consider steady operation. The pulsed detonation engine uses an intrinsically unsteady process of mixing, ignition, deflagration-to-detonation transition, and nominal propagation. The word scenario is used because, at this time to the best of our knowledge, it is probably the case that there is no well-designed and robust detonation engine in operation. Most of the work reviewed describes scenarios, the most important of which is an oblique detonation attached to a wedge; therefore, we will discuss that case in some detail.

Engine operation usually calls for a steady and stable process, so that one assumes, as a starting point, evidence of operational parameters that describe a nominally steady and robust detonation is stabilized by an anchor or control device like a wedge. We will attempt to explain what detonation stability theory might say about realistically achievable two-dimensional, nominally steady detonation flows. However, it must be said that almost all that is known now, and is currently calculable with any scientific certainty, are the stability properties of simplified descriptions of one-dimensional, steady detonations subjected to small disturbances. Very little is known about the detonation stability of systems with complex chemistry, realistic equation of state (for very high pressures), or even two-dimensional flows, for that matter. Information about the application of the linear detonation stability theory to intrinsically multidimensional flow is nearly nonexistent, and the linear theory that could be applied would hold only in some limited domain (portion) of two-dimensional flows.

Most studies of stability that are specifically relevant to propulsion applications have been carried out by computation. That is not an entirely happy state of affairs, because detonations are notoriously multiscale and unstable with sometimes violent transients and thus very difficult to compute with a high degree of accuracy. But we will guide the reader to some of the more interesting attempts to compute stabilized detonation flows. Roughly speaking, what is found by computations is that multidimensional detonation can be stabilized on a wedge by very high degrees of overdrive, that is, the specific kinetic energy of the incoming stream is large compared with the energy released by combustion behind the lead shock. Hence detonation can be stabilized at large freestream flow Mach numbers, with the Mach number cited to be on the order of 8 and above. The theory for detonation linear instability can be used to infer general trends that confirm these simulations, such as that a high degree of overdrive limits to flows of inert shocks in ideal gases, which are at least neutrally stable. But a comprehensive general theory does not exist.

The calculation of stability boundaries by simulation means with a full code, is a very difficult task indeed, because one is trying to compute a bifurcation from stable to unstable behavior, which requires a high degree of both temporal and spatial accuracy. In practical terms, one is trying to compute a zero (or a root as the location of a zero growth rate of a small deviation from a steady solution) in parameter space through the use of a full simulation code. Hence, precise computation of detonation stability boundaries is not done. However, there are works where precisely computed stability boundaries, in the parameter space of a simplified model, have been computed for a one-dimensional steady detonation. In turn, direct simulations of the same have been carried out to confirm the exchange from stability to pulsating instability, because this Hopf bifurcation involves the crossing of a conjugate pair of nonzero frequency, zero growth rate eigenvalues across the imaginary axis, and the pulsations are relatively easy to detect by computation. We know of no cases where 2-D instabilities of one-dimensional steady detonation have been verified in this unambiguous manner, although new (unpublished) efforts are being carried out.

At this time, it is fair to say that other than a definitive picture provided by the analysis of one-dimensional instability of planar detonation, which defines some guidelines for how the stability boundaries are arranged for a simplified geometry for a simplified model, the main contribution of linear detonation stability analysis to propulsion has been its influence on the development of higher accuracy codes. A test of the bifurcation from steady, stable one-dimensional detonation to a pulsating, one-dimensional unstable detonation is now regularly used to test codes and validate them before their use to compute more complex two or three dimensional flows. In this sense, linear stability information defines an asymptotic result for weak amplitude disturbances; that is a very hard and fine test of any code. If the code passes, one feels that it might be trusted to accurately compute flows in other fully nonlinear regimes, where no analytic solution of any type is available. That last statement, however, verifies the accuracy of the numerical formulation, and is not any guarantee of the quality of the simulated results, because that is governed by the properties of the algorithm that experiences specific (nonlinear and varying states) in transient and multidimensional flows. This is a difficult business. However, consider the alternative. Would one trust any simulation code that could not compute a transition from stable to unstable behavior and recover the correct $\mathcal{O}(1)$ oscillation frequency of weak pulsations? Good engineers and scientists would not, hence everyone who writes a proper code, carries out a stability check. The difficulty of this test, and the accuracy, that is, the ability to compute exact values of the unstable growth rates and oscillation frequencies and location of neutral stability boundaries for some simplified models, has surely had a profound impact on improving the accuracy of the numerical algorithms in use today. One uses systematically derived information from stability theory to validate codes and to show consistency in the formulation and/or numerics.

In general, the physical phenomenon of detonation is understood in its details as a multidimensional and time-dependent phenomenon, especially gaseous detonation. In other words, as many before us have noted, one-dimensional gaseous detonation is nearly always observed to be unstable. Other than pulsations, the most manifest instability is due to transverse waves that travel back and forth across the lead shock. As found by experiment, the transverse waves represent a complex of intersecting shock waves that generate shock–shock interactions near and on the lead shock. The lead shock interactions generate well-defined slip lines oblique to the lead shock, trailing back into the reaction zone, and in turn these slip lines ultimately are subjected to slip line (Kelvin–Helmholtz) instabilities. The wave collision process is entirely nonlinear being solely governed by the laws of reacting gas dynamics, not linear stability theory. Linear stability theory at best could play a role in the incipient onset of these nonlinear instabilities, but what is seen in experiment is far removed from linear theory.

Another important aspect of detonation applied to propulsion is ignition. How does one generate a detonation wave from an ignition source? It is fairly safe to say at this point, no one knows (or has identified) any direct correlation between the parameters of stability theory (such as the location of the linear stability boundaries) and description of ignition. Ignition theory is a theory of the transient. The main point is to identify the properties of the ignition source and relate those to a go, no-go criterion; given the source, the material detonates or does not. Experiments with small explosive charges do in fact show a clear energy threshold, and some theory does exist, but it is not related to linear detonation stability properties as far as we know. There indeed may be such connections, but they are not established and hence the links between propagation, ignition, and robust propagation of multidimensional detonation fronts are nonexistent or tenuous at best.

Deflagration-to-detonation transition (DDT) is also a detonation–ignition transient, whereby from a very weak source (a spark, say) a flame that forms in a premixed detonable mixture of gases, by virtue of interaction with self-generated pressure waves that interact with confinement, develops a large amount of flame surface area and the flame undergoes a rapid acceleration. This acceleration produces volumes of burnt gases whose expansion generates more acoustic waves and pressure interaction with the flame, as well as simple adiabatic compression of the mixture far ahead of the flame complex. The process is thought to continue through a bootstrap process of flame/shock interaction until the compression is sufficient to allow autoignition, in a small region of preconditioned and unburnt mixture ahead of the flame brush (the large convoluted deflagrative reaction surface), that subsequently explodes and generates shocks that amplify the strength of the weak amplitude lead shock that appears due to the earlier volume expansion of the products. The strengthening of the lead shock by this process is then sufficient to support detonation.

DDT is only well-described from experiments. The phenomenon involves such a large range of scales that it is very difficult to compute, although there have been some recent attempts to carry out simulations that are true to the experimental scenario described above [5]. There have been some one-dimensional transient simulations of DDT that use lumped piston-like models to describe the compression effects generated by the flame brush. One can safely say there is essentially no satisfactory theoretical description of the entire process, as it is an intensely unsteady and multidimensional process. It is possible to theoretically describe some aspects of subprocesses. There are no reliable occurrences in the literature where results from linear detonation stability theory can be used to interpret the DDT process.

The strongest, nonlinear concept that defines both observed robust detonation phenomena, that is generic to all classes of freely propagating or standing detonation, is the Chapman–Jouguet (CJ) hypothesis. That is, freely propagating detonations observed in experiment are detonations that have a sonic locus behind the lead shock. In the case of steady one-dimensional detonation, the so-called "CJ detonation" is the simplest model, and is selected as a strong detonation in a spectrum of detonations, with a minimum wave speed. In a structureless theory, where the reaction behind the shock is supposed to be infinitely fast (hence the reaction zone has zero thickness), the states across the detonation jump from the ambient unreacted state directly to the burnt state. The CJ-burnt state has its particle velocity exactly equal to the sound speed of the burnt state, hence it is sonic in that steady frame. The real significance of the CJ hypothesis lies in the interpretation of this simple criterion in terms of the space-time characteristics of the steady flow. When the flow is sonic, the forward propagating characteristic (the C_+ characteristic in 1-D, if the detonation propagates to the right) travels exactly at the lead detonation shock velocity. Hence for smooth disturbances, acoustic waves in the burnt region lie to the left (say) of the sonic point, cannot enter into the lead shock and disrupt it. This is the essence of the original CJ hypothesis which is fundamentally a nonlinear stability argument that has its origins in the hyperbolic character of the compressible flow equations that govern detonation.

In both one-dimensional and multidimensional unsteady flows, robust cyclically steady flows are observed. But a variation of this simple CJ hypothesis still holds, and again is rooted in domain of dependence arguments for the governing hyperbolic equations. The sonic point of the steady CJ hypothesis is replaced by a sonic locus, which is simply interpreted in smooth flows as a bounding characteristic surface that separates signals that return to the lead shock from those that flow away from the lead shock and pass their disturbance information into the burnt gases that are swept away. For unsteady detonations that have cyclically, steady limit cycles, this sonic locus moves as well and has a steady cyclical limit cycle. The description of such a limiting sonic locus, necessarily requires the resolution of the reaction zone in a theoretical or numerical representation. Some progress has been made in understanding the stability properties of detonation with embedded sonic surfaces, but even in 1-D, this is a largely unresolved or at best partially resolved problem, even for the simplest models of detonation. Progress has been slowed possibly due to analytic and numerical difficulties associated with the nonlinear and transonic character of the flow near the sonic locus, and those difficulties can be traced back through all the modern work on detonation that started after World War II.

The importance of sonic self-confinement of detonation required for steady, or cyclically steady operation cannot be emphasized enough, and we emphasize this point with a very simple observation of a related (and widely used) propulsion device that uses sonic self-confinement to enable stable, sustained energy release: a solid rocket motor. A solid rocket motor is a pressure containment cylinder filled with solid propellant, that has a ballistic cavity (i.e., a bore hole) down its length, with an attached converging, diverging nozzle at the exit. After ignition from a cold (i.e., unburnt) state, the pressurization of the ballistic cavity and the subsequent quasi-steady burning of propellant and evacuation of the products through the nozzle to produce thrust, entirely depends on the existence of a choked sonic locus in the throat of the nozzle. In cases when flow disturbances far downstream of the motor enter the ballistic cavity (i.e., the nozzle is not choked and the flow there is "subsonic"), then the motor will not pressurize and burn stably. In fact, motors are designed so that choking is inevitable and so that the sonic locus sets up quickly so that the motor can pressurize. Well-designed motors have carefully designed propellant and interior grain shapes that provide a well-controlled energy release as the motor progresses to burn out. Design of the motor attempts to provide an interval, as long as possible, where the motor burns stably on the time scale of the acoustic or material passage through the motor. Sonic confinement is the essential concept in stable solid rocket motor design, and the sonic locus is well-defined relative to the pressure confinement vessel (the "case"), even if the flow is unsteady.

The situation is exactly the same for self-propagating or steady or cyclically standing detonation, both one dimensional or multi-dimensional. The confinement vessel is the lead shock combined with the flow in the subsonic reaction zone that is influenced by lateral confinement, such as a wedge, or in the case of freely propagating detonation in tubes or sticks, confinement provided by side walls or expansion effects. These detonations create their own nozzle, as a stable sonic locus forms in the reaction zone behind the lead shock. The sonic locus is a separatrix (i.e., a surface that moves in space time) for which forward-going (toward the lead shock) disturbances on the upstream side of it can propagate to the shock, but those on the downstream side propagate away from the shock toward the burnt gases. Hence, rocket motors are essentially standing CJ-detonation waves, where the lead shock that provides the confinement is replaced by the pressure vessel in which the energy release occurs.

There is a substantial body of theory that deals directly with multidimensional CJ detonation, that of detonation shock dynamics, for simple models of detonation, derived both for gases and for application to condensed phase explosives (see the recent review by Bdzil and Stewart [6]). This asymptotic theory presupposes a weakly curved detonation, for which the radius of curvature of the lead detonation shock is large, compared with the width of the reaction zone that lies behind the lead detonation shock, and that changes in shape of the lead detonation shock take place on a time scale that is long compared with the transit time of a particle that passes through the reaction zone; hence a quasi-one-dimensional, quasi-steady theory is assumed. A sonic locus is assumed to be embedded in the reaction zone, and it is a consequence of both the curvature and the reaction. From those assumptions it is possible to systematically derive evolution equations for the lead shock motion, whereby the shock location and its dynamics are entirely determined by the intrinsic shape and dynamics of the lead shock, subjected to lateral boundary conditions that represent confinement.

Although such theory has been used extensively and successfully to study detonation in condensed explosive systems, we are unaware of any systematic attempt to use these types of analysis in the application of the detonation of gaseous explosive mixtures to propulsion. However, the essential nonlinear concept of sonic confinement associated with the CJ detonation, is common to both condensed phase and gaseous phase detonation applications. It is possible to generate approximate evolution equations that are numerically shown to develop cellular instabilities on a lead shock akin to those seen in experiments in gases at low pressures and low fuel concentrations. This analysis is promising but incomplete.

Theoretical formulations exist for multiphase detonations that are based on the concept of coexisting phases, and use the constructs from continuum mixture theory [7]. For pulsed detonation applications, one considers a gaseous oxidant phase and a fuel droplet phase, nominally from an aerosolized light hydrocarbon jet fuel like JP-4. The relevant multiphase theories can be quite complex in their formulation as two sets of transport equations are required for both phases (liquid and gas, or solid and gas, say), and various coupling terms must be provided in the theory that account for interphase exchanges of mass, momentum, and energy. Additional closure assumptions must be made to complete model specification like pressure and temperature equilibrium, or specified disequilibrium. Even one-dimensional models are notoriously complex and not straightforward to compute. For example, in a one-dimensional problem with a single reaction decomposition of fuel to product, one has four equations, with three real characteristics. For the simplest one-dimensional multiphase theory one has at least eight equations, with at least six real characteristics, if the chosen closure allows the system to be hyperbolic. Most of the work carried out has been that of formulation, steady solutions and numerics. There are no reliable theoretical results for detonation stability for this class of models that we know of.

Next, in Sec. II we give a succinct review of the theory of detonation instability. We review the state of the theory of detonation instabilities, starting with the conclusions obtained from two-dimensional numerical simulations over wedges and blunt bodies. These detonation flows are directly related to propulsion devices and to date have not been directly addressed by theory. Then we discuss selected contributions from the theory of planar detonation instabilities from its earliest formulations, starting with Erpenbeck to recent contributions. Various asymptotic treatments, that include both activation energy asymptotics, weak curvature, and slow temporal evolution, lead to reduced descriptions of the detonation dynamics and evolution equations for the front, that in turn have reduced stability descriptions; we include a description of these results. We discuss aspects of direct initiation of detonation from concentrated energy sources and the relation of the ignition and propagation transients to stability theory. In Sec. III, we give the basic normal-mode analysis that forms the basis of the standard theory, and show some representative results. In Sec. IV, we list some outstanding research issues and conclusions.

II. State of the Theory of Detonation Instabilities

A. Nonlinear Stability of Detonation Flows over Wedges and Blunt Cones

Detonation structure generated by a wedge inserted in a uniform unreacted stream of explosive gases is a two-dimensional flow that has been studied extensively by numerical computation. In the literature this configuration is referred to as an oblique detonation wave (ODW). The configuration is a fundamental one that is fairly simple to simulate and is relevant to hypersonic air-breathing propulsion schemes [1,8]. Much of the published work considers premixed mixtures of hydrogen, oxygen, and diluent.

There are no exact two-dimensional solutions of which we are aware, except for the single exception found in the works of Powers and Stewart [9] (analyzed in a weak-heat-release, hypersonic limit), and a later update by Powers and Aslam [10] (where the equations of the steady flow are integrated exactly for general conditions). In this case, a curved wedge configuration provides confinement for an oncoming uniform, premixed flow, and the post shock, confining wall of the wedge is curved so as to precisely adapt to particle motion that occurs due to expansion of the gases in the detonation reaction zone. Hence the lead shock is straight, and the steady streamlines in the reaction zone are curved, parallel, and conform to the wedge shape. Because the shock is flat, the steady flow behind the shock is irrotational. This is a very special solution indeed, because the geometrical configuration required by the confining wedge depends on both the inlet conditions and the mixture conditions of the premixed fuels. To maintain the flat shock shape in an engine with changing operating conditions would require continuous changes in the shape of the curved wedge. Whether or not this is a practical configuration for engine design is not clear, but this special solution is an unambiguous and realizable two-dimensional exact solution and hence could be amenable to further analysis. Powers and Aslam make the strong case that this solution is invaluable for verification purposes of hydrocodes. The reader is referred to Powers' review in this journal issue [11], where he gives a full account of comparisons of simulation against this exact solution.

For both the straight wall wedge, or for Powers et al.'s special solution of the flat shock, curved wedge, the formulation of a stability problem for a steady two-dimensional detonation has not been posed, unlike that for the plane steady detonation. Therefore, the issue of stability of detonation flow over a wedge has been studied entirely by numerical simulation. Fujiwara and colleagues carried out early simulations of ODW [12]. Li et al. [13] demonstrated that a steady oblique detonation could be established on a wedge, and that a critical wedge angle existed where the detonation structure would detach from the anchor point at the wedge turning corner, similar to inert flows. This wedge angle was associated with sonic flow behind the lead shock which can be identified from the shock polar analysis. They showed that under many conditions the basic structure of the oblique detonation consisted of the oblique shock that initiated reaction, with a subsequently well-defined induction region followed by a reaction region along the wall. Papalexandris [14] shows examples of these basic flows at the highest resolution we found in the literature, where the details of the structure are clear, and provides comparisons with other works. Because of the confinement provided by the wedge, the exothermic energy release in the nominally steady supersonic flow region behind the lead shock, generates compression waves which propagate on the forward acoustic characteristics to form a shock downstream off the wedge. This compression event generates a triple point with incident, reflected and Mach stem shocks. The reflected shock extends into the fresh mixture at an angle more normal to the flow, and thus the compression across this portion of the lead shock is higher than that for the incident oblique shock. Subsequently, the reaction zone behind the reflected shock results in a detonation that has a much shorter reaction zone than that for the oblique incident shock. The Mach stem and reflected shock align themselves so that the slip line runs approximately parallel to the downstream wedge. A schematic of a nominally steady flow configuration is shown in Fig. 1. (In many works, the Mach stem is not shown as part of the schematic.)

Very high inlet speeds and small wedge angles are found to generate stable solutions. Grismer and Powers [15] show computed, stable solutions and comparison with the asymptotic steady solutions attained in a hypersonic (weak heat release) limit [9]. Relatively weak heat release at very high inlet enthalpies results in the compression waves from reaction behind the incident oblique wave that are no more than sound waves associated with an acoustic compression, and turn the lead, reflected shock without formation of

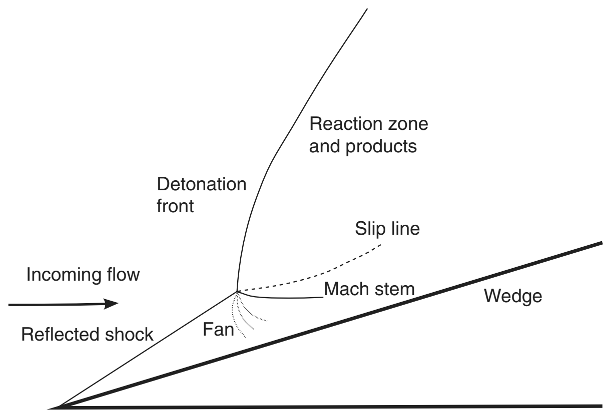

Fig. 1 Schematics of the oblique detonation wave stabilized on a wedge.

the triple point. Simulations by Li et al. [13], Thacker and Chelliah [16], Grismer and Powers [15], Lefebvre and Fujiwara [12], Papalexandris [14], Da Silva and Deshaies [17], Fusina et al. [18] show evidence of sustained pulsation of the wave complex on the wedge as the exothermic heat release is increased relative to the incoming enthalpy of the inlet flow, or as the activation energy is increased. Studies with complex chemistry [16,18] show qualitatively similar results to those carried out with simplified one-step chemistry [14,15].

In summary on review, we find that the wedge configuration is fundamental in nature, is accessible experimentally, has all the essential nonlinear gas dynamic elements associated with transverse wave instabilities for planar detonation, has demonstrable flow configurations that are both stable and unstable, but has not been analyzed to any significant extent by theoretical means, other than by numerical simulation. Approximate simple wave analysis does not account for observed distribution of reaction, despite the basic simplicity of this flow. Next we turn to a discussion of the theory of detonation stability for planar detonations.

B. Summary of the Theory of Detonation Instability for Planar Detonation

1. Exact Treatments of the Basic Model

Here we provide a concise summary of the state of the theory of planar detonation instabilities. Although there are predecessors, the modern theory of detonation stability starts with the work of J. Erpenbeck at Los Alamos National Laboratory who from 1962 to 1970 wrote an interconnected series of 13 articles (eleven of which appeared in the fairly young journal *Physics of Fluids* and two in the *Proceedings of the Combustion Institute*), that laid out the entire framework of the current theory for the basic detonation model for a mixture of premixed explosive gases. The period from late 1950s to mid 1960s was a time when fuel–air explosives were being studied extensively and key early experimental observations of transverse structure in gaseous detonation were obtained by Voitsekhovskii et al. [19,20], Denisov, Shchelkin, and Troshin [21,22], Duff [23], White [24], Schott [25], Strehlow [26], Soloukhin [27], and others. Fickett and Davis [28] describe the state of understanding of detonation theory and detonation stability theory and provide an extensive bibliography of works through 1979 (including Erpenbeck's papers).

Erpenbeck's model, upon which his stability work is based, is for a premixed ideal gas with a first order irreversible reaction $A \to B$. In Sec. III we present details for this basic model. His results are recorded in papers [29–35]. In his 1962 article [29], Erpenbeck posed the basic time-dependent problem and the stability problem in a lead, shock-attached frame. The stability problem is properly viewed as an initial-value problem for small disturbances from the steady state governed by the linear approximations. He used the Laplace transform to replace time and then formally solved the spatial ordinary differential equations (ODEs) in the structure to obtain a relation for the transformed shock displacement amplitude, which arose from both the linearized lead shock relations and the shock acceleration terms. By placing a boundedness condition on the solutions for the disturbances in the equilibrium region of the leading order (steady) solution, he obtained a formula for the Laplace transform of the shock displacement that in turn was represented as the ratio of two analytic functions in the transform variable, of the form $U(s)/V(s)$, where s is the transform variable. The Nyquist winding theorem was then used to define a numerical procedure that for a given set of parameters that defined a plane detonation of interest, would determine the zeros of $V(s)$ in the complex s plane. The function $V(s)$ was, of course, defined by various integrals of the steady-state structure from the shock to the end of the reaction zone. The Nyquist winding theorem required the evaluation of these integrals along a large semicircular contour in the right half s plane; and if zeros of $V(s)$ were located in the right half s plane, then the winding integral procedure would compute the number of zeros that corresponded to exponentially unstable pole solutions, hence instability. In his 1964 paper [31], Erpenbeck worked out this procedure for the basic model and determined approximate locations of neutral stability boundaries by varying parameters to bracket the locations of boundaries in parameter space. These parameters included the overdrive factor, $f = (D/D_{CJ})^2$, the transverse wave number k, the Arrhenius activation energy E, the heat-release Q, and so on. The procedure was correct and exact, albeit entirely numerical, and indeed later in other papers he bracketed roots so finely [34,35] (where Erpenbeck considered weakly nonlinear one- and two-dimensional instabilities) that he could then go back with those values to determine eigenfunctions and growth rates. But because only pole solutions were sought and could be attained by searching for the zeroes of $V(s)$, and because the determination required a cumbersome "by hand" iteration of the locations of poles, it is fair to say that the simplicity of using a straightforward normal modes approach was overlooked in all this work. After Erpenbeck's 1970 paper [35], no significant work that used the exact formulation of the basic model is found until the early 1990s with the work of Lee and Stewart [36], and Bourlioux and Majda [37] of which we will say more below.

In their 1966 paper, Fickett and Wood [38] carried out a one-dimensional simulation of pulsating overdriven detonation and showed the transition from stability to instability via a Hopf bifurcation, with the correct oscillatory frequencies as predicted by Erpenbeck's stability calculations. Also this work demonstrated that the onset of instabilities is measured on time scales that are of the order of the particle transit time across the reaction zone. This work established the correct scaling for observance of regular pulsations, similar to those recorded in the experimental work of Lehr [39] in the early 1970s that observed oscillatory instabilities that originated near the nose of hypersonic projectiles launched into stoichiometric hydrogen–oxygen mixture. To our knowledge, this was the first demonstration where both the stability growth rates and eigenfunctions were used to verify direct numerical simulation and vice versa. This type of verification has become a principal requirement of any simulation code used today.

Erpenbeck's 1963 paper [30] is one of the early uses of large activation energy asymptotics to study combustion problems. In that paper, Erpenbeck constructs the asymptotic solution for the induction zone with $\mathcal{O}(1/E)$ reaction depletion and then posits a fire (an instantaneous) reaction at a finite location from the shock. The one-dimensional stability of the square wave with a discontinuity fire zone then exhibits a pathological spectrum that is associated with the lack of structure in the fire zone. This pathology was later resolved by exact normal-mode treatments found in Lee and Stewart [36] and Short's work on the large activation energy limit [40], both of which show that at large enough temporal frequencies the spectrum is stable. Again, we will say more about this below.

In his 1966 paper [33], Erpenbeck claimed to show using asymptotic arguments that disturbances with high transverse wave numbers are unstable whereas those with low wave numbers are stable, and gives a simplified criterion based on the shape of the sound speed squared (i.e., the temperature distribution). This conclusion and criteria was later discussed in 1995 by Bourlioux and Majda [41], possibly as the basis for a theory of ray trapping and amplification of acoustic disturbances based on high-frequency asymptotics. However, exact numerical computations of the spectra by normal modes now show that the high wave number spectrum is stable, hence Erpenbeck's conclusions are in doubt. Finally, regarding Erpenbeck's work on weakly nonlinear stability theory as explained in the 1967 and 1970 paper, Majda and Roytburd [42] argue that this original attempt by Erpenbeck used an ad hoc assumption in the asymptotics and did not use the full adjoint problem in the asymptotic closure. A formulation for the weakly nonlinear stability of both one and two-dimensional overdriven detonation that remedied this problem was presented in the papers of Bourlioux, Majda, and Roytburd [41,42].

As mentioned above, Erpenbeck's formulation was invaluable, and most of his works have subsequently been found to be correct, but the original procedures used for analysis of the pole solutions of the Laplace transform of the linear disturbance partial differential equations, which are simply the normal modes, may have impeded subsequent progress. In a 1987 conference [43], one of the authors gave an overview talk discusssing the unsatisfactory state of affairs of the detonation stability theory. One of the outcomes of that workshop was that at Illinois we developed a direct and simple-to-implement method that solved the stability ODEs directly and found a procedure that directly generated the dispersion relation [36]. In particular, we were able to simply generate eigenvalues and eigenfunctions and find neutral stability curves by straightforward continuation methods in parameter space. Importantly, it was shown that the case of a Chapman–Jouguet detonation could be obtained by taking the limit as the overdrive factor $f \to 1$ and so that limit was not singular.

Subsequently, Bourlioux [37] developed a high quality numerical integration procedure for the Euler equations and verified transition from stability to instability as predicted from now precisely computed spectra for the stability problem . The newly identified procedures and methodologies for exact treatment of the stability problem and high quality numerics developed in the early 1990s have become basis and standard of comparison for many of the detonation stability studies carried out since then. In particular, approximate theories that have been developed to elucidate mechanisms and generate approximate spectra can be checked against spectra and eigenfunctions computed exactly. A discussion of the basic problem is described in Sec. III.

Notable exact treatments of the basic model are found in works of Short [40] and Short and Stewart [44] where a detailed numerical investigation of the spectra for both overdriven and CJ detonations are presented. In his 1997 paper [40] Short, by numerical means, investigated the one and two-dimensional linear instability for intermediate and very large activation energy and compared his results with asymptotic theories for square-wave detonation (discussed below). He has conclusively shown that whereas for large activation energies the one-dimensional spectrum has many unstable roots, that it is not pathological in the sense of the discontinuous square-wave model treated earlier by Erpenbeck, and that for sufficiently high frequencies (mode numbers) the spectrum is stable. In their 1998 paper [44], Short and Stewart show conclusively that short wavelength stability prevails in contrast to Erpenbeck's results. They also display results for how the group velocity varies with wave number and show from the exact spectra that the group velocity in a band of unstable wave numbers is maximum at low wave numbers, and lower than the wave number with maximum growth rate. This was offered as a possible explanation that detonation cells that initially are observed to develop at the wave number with the maximum growth rate, grow and migrate toward larger sizes and hence lower wave numbers. This followed a similar proposal made for the dispersion relation obtained for an asymptotically derived evolution equation discussed by Stewart et al. [45]. Sharpe [46] extended the asymptotic description of the disturbances at the end of the reaction zone for the CJ detonation, and recovered same results found in Lee and Stewart's [36] treatment as $f \to 1$.

In 1997 Short and Quirk [47] introduced an extension of the basic model and considered a reaction model that has a sequential chain initiation and chain-branching steps governed by Arrhenius kinetics and a temperature independent chain-termination step. This model results in a temperature sensitive induction zone with a temperature independent main reaction zone and has one additional degree of freedom over a single irreversible reaction. They carry out an exact stability analysis for this model verified by illustrating onset of instability and bifurcation of dynamical behavior associated with a crossover temperature that controls the relative length of the induction and recombination zones.

Sharpe [48] used an exact normal-mode approach to investigate the linear stability of the so-called "pathological detonations," with a multiple step scheme $A \to B \to C$, in which the first step is exothermic, whereas the second is endothermic. This leads to the possibility of a sonic point in the reaction zone at partially completed reaction. He proposes two possible steady structures past the sonic point flow; one has a continued expansion and is supersonic, and the other is a compression that is subsonic and must be associated with a piston support. The latter is not known to be observed experimentally as far as we know. Sharpe concludes that results for stability for the pathological (sonic) detonation do not depend on the post sonic point steady structure, as to be expected. This paper does not offer any numerical confirmation of the results.

Kasimov and Stewart [49] carried out an exact treatment of detonation instabilities in circular tubes. They develop neutral stability curves in the plane of heat release and activation energy and exhibit bifurcations from low-frequency to high-frequency spinning modes as the heat release is increased at fixed activation energy. With a simple Arrhenius model for the heat-release rate, good agreement with experiment is obtained with respect to the effects of dilution, initial pressure, and tube diameter on the behavior of spin detonation. Again, no independent verification of these results by direct numerical simulation has been reported on at this time.

2. *Asymptotic Treatments of the Detonation Stability Problem*

Because the structure of a steady detonation involves variation in the states that is determined by the functional form of the energy release rate, the leading order (steady) solution cannot generally be expressed in terms of elementary functions and the linearized system of differential equations of stability theory has nonconstant coefficients. A notable exception to this is the square-wave model approximation to the structure of a detonation, considered by Zaidel [50] and later by Erpenbeck [30], but as we have seen, that model is ill posed with the remedy that one must consider the continuous structural variation in the reaction zone, instead of piecewise constant structure. Therefore, since the inception of the stability problem, many researchers have sought approximate and asymptotic solutions to compute the stability spectra of detonation instabilities. Erpenbeck's treatments were formulated as exact treatments, with the exception of his work on the square-wave detonation for which he recorded difficulties. His other work used asymptotics only in regard to the character of the dispersion relation (i.e., his work on the high wave number limit), or in his attempts to derive evolution equations for weakly nonlinear evolution for detonation with parameters whose values are near neutral stability boundaries. These are still regarded as exact treatments.

a. Approximate Treatments of Toong and Coworkers. In the 1970s and 1980s Toong and coworkers [51–54] carried out a series of experimental and theoretical studies to elucidate mechanisms of detonation instabilities. Quoting from Stewart's previous paper with Lee [36], pps. 118–199:

> In 1971 and 1972, McVey and Toong, and Alpert and Toong, published studies of the detonation instability observed when blunt projectiles are fired at high speed into detonable gases. There, they elaborated a wave-interaction mechanism to describe the observed longitudinal instability, which relies on the existence of an induction zone behind the lead shock. The essential ingredient . . . is that temperature perturbations created by acoustic disturbances reflecting off the shock and the reaction zone, change the induction

> time and cause dramatic movement of the reaction zone forwards and backwards relative to the shock. From the experiments they were able to show that the periods of oscillation were … proportional to the chemical induction time in the hydrocarbon–air, hydrogen–oxygen mixtures. … to theoretically predict … the wave-interaction mechanism … Abouseif and Toong [53] gave an approximate [normal modes] linear stability analysis … with ad hoc approximations justified by arguments for large activation energy but not made by systematic asymptotic approximations.

Although the ad hoc treatments for computing the unstable spectra are now in a sense obsolete, they were important contributions that further confirmed that pulsating instability occurred on the induction zone time scale, consistent with experiment and consistent with the previous theoretical and computational findings of Erpenbeck and simulations of Fickett and Wood.

b. Asymptotic Treatment. The use of rational asymptotic approximations is employed for two reasons: 1) to elucidate essential mechanisms and 2) to generate useful reduced descriptions of the phenomenon. It is also fair to say that other than the notable work of Bdzil [55,56], until the late 1980s asymptotic methods had been used sparingly to understand detonative phenomena, and it is fair to say, not at all for understanding detonation instabilities. This stood in stark contrast to the striking developments and accomplishments that used rational asymptotic methods to describe low Mach number combustion that started in the late 1960s, with the work of A. Linan, J. F. Clarke, and many others that have continued through to the present.

Numerous asymptotic limits are available to analyze gaseous detonation for the basic model of Erpenbeck and its variations. Parametric limits include the limit of large activation energy, $E \to \infty$, the limit of small heat of combustion, $Q \to 0$, the Newtonian limit, $\gamma \to 1$, the limit of large overdrive, $f \to \infty$, the limit of near-CJ detonation, $f \to 1$. Other limits are defined in terms of the state of the flow and its spatial and temporal variations, and they include the limits of slow temporal variation (the quasisteady approximation) $\partial/\partial t \sim \mathcal{O}(1)$, weak transverse variations or weak lead shock curvature (the quasi-1-D approximation), $\kappa \to 0$, high-frequency limits, $k \to \infty$, and so on. Of course, the stability problem itself is an asymptotic analysis of an initial-value problem for data defined close to a base state, valid for time $t \sim \mathcal{O}(1)$ and can only be understood properly as such. Distinguished limits consider combined limits controlled by one parameter. Successive limits consider parameter or coordinate limits in succession. Most of these limits were examined in various forms by numerous researchers and we will attempt a brief explanation of some of the important contributions that bear on the question of stability.

3. *Large Activation Energy Asymptotics*

The limit of large activation energy, applied alone, is a very difficult limit due to the fact that the induction zone becomes very long, and the reaction, when it occurs, is exponentially thin compared with the induction zone. This leads to exponentially sensitive dynamics. Indeed, treatments of the exact problem [36,40] show that for increasing activation energy, a tremendous number of unstable modes are available to most planar detonations, all other parameters staying fixed. In 1986 Buckmaster and Ludford [57] carried out an asymptotic analysis that considered long transverse wave length disturbances and slow temporal variation, both $\mathcal{O}(1/E)$ in the limit of large activation energy, for the basic problem. They found an unstable nonoscillatory root and concluded that in this limit detonation is always unstable. Later Buckmaster and Neves [58] revisited one-dimensional stability for the limit $\partial/\partial t \sim \mathcal{O}(1)$ and that spatial variation of the perturbations are on the order of the induction zone in the large activation energy limit, and obtained the pathological spectra (increasing instability with increasing frequency) as reported earlier by Erpenbeck. In 1996 Short [59] developed one- and two-dimensional results for combined limits of large activation energy and the Newtownian limit analyzed by Blythe and Crighton [60] for shock generated ignition. Short found a reduced asymptotic expression for the modes that are consistent with the exact numerics. He also found the pathological features of the one-dimensional high-frequency spectra, consistent with the finding of Buckmaster and Neves. Later, by comparison of the asymptotics with exact computation of the one-dimensional spectra [40], Short resolved the pathological dilemma by computing the spectra for extremely large activation energies, much larger than any previous researchers had considered, and showed that at high frequencies, hence on scales much shorter than the induction zone time, the spectrum is stable. The asymptotic analyses were only valid for $t \sim \mathcal{O}(1)$ measured on the induction time scale and are not valid for the high-frequency portion of the spectrum.

Yao and Stewart [61] used asymptotics based on near-CJ detonation with weak shock curvature, and slow evolution based on reaction zone length and time scales, to develop a reduced dynamical description of an evolving near-CJ detonation for the basic model. They analyzed the problem in an intrinsic shock-attached frame, such that both the shock acceleration and the shock curvature (via the flow divergence) appeared in the governing equations. For the rear confinement condition at the end of the reaction zone, they applied a quasisteady sonic condition. Because the curvature and time-dependent terms in the governing equations were deemed small, those terms were placed on the right hand side, and a formal integration through the reaction zone structure obtained integral equations that are tractable. They were able to approximate the dynamics using the method of successive approximations to generate multiscale asymptotic approximations. The first nonplanar correction to the structure generated normal detonation velocity curvature relation and the higher order iterations brought in corrections that included the normal detonation velocity, normal shock acceleration, the normal time derivative of the shock acceleration, the curvature and the normal time derivative of the curvature. The asymptotic ordering was chosen in such a way as to ensure that modal truncation led to evolution equations that had well-posed evolution; hence, a hierarchy of evolution equations was obtained. Because this procedure requires the evaluation of the integrals on the right hand sides of the governing equations, the large but finite activation energy limit was used to get explicit expressions. At the final order of truncation, a third order in time, second order in space hyperbolic nonlinear partial differential equation for lead shock motion was obtained. Subsequent numerical solution (with Aslam) showed that for parameters that were reasonable facsimile for the dilute hydrogen–oxygen mixture, this shock evolution equation admitted both one-dimensional pulsating instabilities and cellular instabilities that produced large, saturated cells whose width was far larger than the corresponding induction zone length.

In their 1997 paper [45], Stewart, Aslam, and Yao developed the reduced linear stability theory for this evolution equation. One deficient feature of the reduced dispersion relation (which was third order in the growth rate and second order in the wave number) was that, although there was instability that led to the growth of large cells, there was not a maximum in the growth rate that identified the linearly unstable cells that are a feature of exact stability theory; this deficiency is associated with the truncation of terms in the approximation scheme and is not inconsistent with the inherent low wave number assumption. However, the dispersion relation does exhibit a maximum in the group velocity, and like the Kelvin's explanation for ship wake patterns [62], it was suggested that the cell size in the simulation of the front evolution equation might be selected by the maximum in the group velocity. Motivated by observations of experiments and simulations that the instabilities captured in low-frequency spectra seem to be conveyed to large amplitude nonlinear detonation dynamics, a careful examination of the low-frequency spectrum was carried out by Short and Stewart [63]. A similar examination of the weak-heat release and large overdrive limits is recorded in their 1999 paper [64] and regimes are identified where there is a single band of wave numbers with unstable wave length.

Using similar limits as Yao and Stewart, Short [65] derived a linear evolution equation that retained higher order terms than that of Yao and Stewart. The resulting evolution equation is third order in time and sixth order in space and is parabolic (as opposed to hyperbolic) in character. Analysis of the dispersion relation showed that this higher order result, in fact, does recover a maximum growth rate and has a limiting wave number above which all disturbances decay and hence removes the deficiency of the lower order truncation.

Asymptotic analyses by Clavin and He and coworkers [66–71] mainly deal with combined limits of large overdrive, weak heat release, the Newtonian limit, and strong rate sensitivity (these authors argue against studying the basic one-step Arrhenius model and instead consider general forms). For the Newtonian limit, the acoustics is simplified and the pressure is nearly constant, hence the limit is also known as the isobaric limit. Consequently, one obtains equations for the temperature and the mass fraction at the leading order correction to the constant state, and can integrate those perturbations on the material (entropic) characteristic and thus introduces a delay, once the shock and rear boundary conditions are imposed. Hence the effects of acoustics are minimized in this limit. Clavin and Denet [70] obtain an integrodifferential delay equation that governs the overdriven detonation shock front, and present numerically obtained solutions that indicate the development of cells, not unlike those found by Yao and Stewart [61] for near-CJ detonation for the basic model. In most of this work no comparisons are made of the reduced spectra obtained by their analysis and exact spectra or with numerical simulation, or physical experiment, as far as we have been able to determine by careful reading.

C. Comparison with Numerics and Computational Requirements

As mentioned previously, the original comparison of the results of direct numerical simulation with exact results computed from linear stability theory for the basic model, was due to Fickett and Wood [38] in 1966. That calculation was a special and remarkable one for its time because it was based on the full method of characteristics, and in some sense was hand crafted. Fickett and Wood literally solved the problem with a computer assisted characteristic net that they continuously iterated on by stopping the calculation and then restarting it with new characteristics added (located more or less by hand) as they noticed the resolution deteriorating, in an iterative fashion.* Since then many researchers have computed the pulsating overdriven instability for the original Erpenbeck–Fickett–Wood test case for pulsating one-dimensional detonation, as well as many other 1-D cases, once abundant information about the linear stability normal modes became available in the early 1990s. Notably, Bourlioux et al. [37] were the first of the group in the early 1990s that recomputed one-dimensional linear stability and transition to instability as a verification of both direct numerical simulation and the exact normal-mode analysis. One finds 1-D simulations of pulsating overdriven detonation for verification of the code used to simulate 2-D, reactive flow over a wedge, for example, in [13,15]. Simulations of one-dimensional detonation dynamics have been the subject of a significant number of studies [46,47,72]. Some interesting new work looks at the issue of bifurcation from pulsation and transition to chaos [73], and the issues associated with elimination of shock generated errors by computing in a shock-attached frame [74,75]. There are numerous other papers not listed here that have computed the 1-D pulsation.

In their 1992 paper [76], Bourlioux and Majda showed that for some selected cases of the basic model, the wavelength with maximum growth rate, as predicted from linear stability theory, was observed to initially emerge as the dominant disturbance in the initial transients computed by direct numerical simulation in fairly narrow channels with lateral periodic boundary conditions. The Bourlioux–Majda numerics featured a finely resolved zone in the vicinity of the lead shock. Sharpe and Falle [77,78] carried out similar computations with an adaptive mesh refinement code and reported similar results, and carried out a resolution study of nonlinear structures observed when transverse waves are present. They argue that the resolution for computing accurate early time detonation dynamics and transition from stability to instability requires on the order of 50 cells per steady half-reaction length or higher. Sharpe argues [79] that, in the context of one-dimensional pulsations, simulations with an adaptive mesh refinement code show that initially regular oscillations are modulated at very long times. Short and Quirk reported the need for very highly resolved calculations (hundreds of points in the reaction zone) in their one-dimensional studies for the transient computation for chain-branching kinetics [47]. Bdzil et al. [80] and Stewart et al. [81] also report (in the context of condensed explosive applications) the need for an absolute minimum of many tens of points in a nominally steady reaction zone structure to ensure accurate calculation. It is fair to say at this point in time, that whereas linear theory has been verified in a few cases by multidimensional direct numerical simulation, there have been no verified two-dimensional simulations because the computational requirements can be massive even if adaptive mesh refinement techniques are used.

*Wildon Fickett, Los Alamos National Laboratory, private communication to D. S. Stewart, 1988.

D. Direct Initiation of Detonation and Its Relation to Detonation Stability

Numerous investigators have examined both criteria and the dynamics of direct initiation of detonation from planar, cylindrical, and spherical sources. The question of direct initiation of detonation is especially important for propulsion applications [82–86]. One of the basic simulations takes a blast wave of known strength and uses a direct numerical simulation code to compute the transients associated with the decaying blast-wave transmission into the explosive mixture and the ignition or failure of a resulting detonation. The transient reflects an overdriven detonation whose shock decelerates and undershoots the Chapman–Jouguet velocity for a planar detonation, often followed by a reacceleration. The recent work [85,87,88] emphasizes the importance of retaining unsteady effects in the development of any direct ignition criteria. It is likely that this transient relaxation and drop of shock velocity through CJ followed by the reacceleration is related (or at least highly correlated) to the lowest frequency modes of the CJ solutions similar to the onset of galloping detonation. But this assertion has not been explored in any systematic way, at this time. However, the ignition transient for the start up of a detonation and its stabilization is, in fact, a central question that must be answered for successful operation of a propulsion device that employs a detonation, and so we believe this is an important issue that must be explored further.

III. Basic Theory

Steady, planar [one-dimensional (1-D)] detonation is the simplest form of detonation and its description provides the fundamental basis for the prediction of much of the observed phenomena in experiments. The system of reactive Euler equations is the model for the physical system and its 1-D solution, commonly referred to as the ZND (Zel'dovich-von Neumann-Döring) solution, is fairly simple in form, satisfies algebraic relations, and is, at most, a system of ordinary differential equations, which in turn describe the chemical kinetics that allows for distributed heat-release behind a lead detonation shock. With fairly simple assumptions about the equation of state and the reaction rate law for the explosive mixture, the predictions of the steady theory are in fair to excellent agreement with gross features of experiment. The evolution of small perturbations to the 1-D steady detonation wave structure is the one most studied. Subsequently, the analysis of detonation stability based on the study of the linearized equations that describe the perturbation theory from this simplest, exact steady solution largely forms the bulk of the stability theory verified by scientific computation.

We start by reviewing the formulation for 1-D steady detonation stability. The model and formulation is the same as that used by Erpenbeck [31]. Our notation will mostly follow that introduced by Lee and Stewart [36] and Bourlioux, Majda, and Roytburd [37]. The equations that follow are dimensional unless stated otherwise.

A. Governing Equations

The standard model assumes that explosive mixture can be described by an equation of state for the mixture $e(p, v, \lambda)$ and a reaction rate law of the form $\omega(p, v, \lambda)$. The primitive variables are taken to be $\boldsymbol{q} = [v, u_1, u_2, p, \lambda]^T$, where $\boldsymbol{q}$ is a 1×5 column vector.

The simple model for an ideal gaseous explosive has $e = pv/(\gamma - 1) - Q\lambda$ where γ is the ratio of specific heats and Q is the heat of combustion. The simple model can be generalized to a nonideal model that includes N independent reactions with mass fractions λ_i, reaction rates $\omega_i(p, v, \lambda_1, \ldots, \lambda_N)$ with a caloric equation of state of the general form $e(p, v, \lambda_1, \ldots, \lambda_N)$. Generally, one supplies a thermal equation of state that defines the temperature T, illustrated here by the ideal gas law for a simple mixture, $pv = RT$. In this formulation, the temperature is not needed as a fundamental variable, but is regarded as an auxiliary variable.

For an explosive described by $e(p, v, \lambda)$ and $\omega(p, v, \lambda)$, the governing equations in the primitive variables are written as

$$\frac{Dv}{Dt} - v\nabla \cdot \boldsymbol{u} = 0, \qquad \frac{D\boldsymbol{u}}{Dt} + v\nabla p = 0$$
$$\frac{Dp}{Dt} + \rho c^2 \nabla \cdot \boldsymbol{u} = \rho c^2 \sigma \omega, \qquad \frac{D\lambda}{Dt} = \omega \tag{1}$$

where $c^2 = v^2(e_v + p)/e_p$ is the sound speed squared and $\sigma = -e_\lambda/(e_p \rho c^2)$ is the thermicity (subscripts in e denote partial differentiation). For the ideal gas, one has $c^2 = \gamma pv$ and $\sigma = (\gamma - 1)Q/c^2$. For simple depletion with Arrhenius kinetics, one has $\omega = k_\omega (1 - \lambda) e^{-E/(pv)}$.

B. Shock Relations

The unsteady shock relations define the states at the shock. For an unsteady detonation, the detonation shock velocity can be specified by $\boldsymbol{D} = D_n \boldsymbol{n}$, where D_n is the normal shock velocity and $\boldsymbol{n}$ is the normal unit vector to the shock, $\boldsymbol{t}_i$, with $i = 1, 2$ are the unit tangent vectors to the shock. The lead shock relations for a reactive mixture that is unreacted and motionless ahead (denoted by subscript 0, whereas subscript s denotes the shock state), can be specified as

$$\rho(\boldsymbol{u} - \boldsymbol{D}) \cdot \boldsymbol{n}|_s = -\rho_0 D_n \equiv \mathcal{M}, \qquad p_s - p_0 = \mathcal{M}^2 (v_0 - v_s)$$
$$e(p, v, \lambda)|_s - e_0 = \tfrac{1}{2}(p_s + p_0)(v_0 - v_s), \qquad \boldsymbol{u} \cdot \boldsymbol{t}_i|_s = \boldsymbol{u} \cdot \boldsymbol{t}_i|_0$$
$$\lambda_s = 0 \tag{2}$$

C. One-Dimensional Steady Solution

One assumes that the steady detonation travels at speed D in the positive x-direction (say), into the ambient motionless atmosphere with upstream states $\boldsymbol{q} = [v_0, 0, 0, p_0, 0]^T$. Introduce the shock-attached coordinate n, defined by $x = n + Dt$, where D is the steady plane shock speed. The conservative form of Eqs. (1) can be used to simply construct the 1-D, ZND solution as follows: Let $U \equiv u - D$, then integration of the conservative form of the mass, momentum and energy equations (not shown) leads to the following algebraic (Rankine–Hugoniot) relations that hold throughout the structure:

$$\rho U = -\rho_0 D \equiv \mathcal{M}, \qquad \rho U^2 + p = \rho_0 D^2 + p_0 \equiv \mathcal{P}$$
$$e + pv + U^2/2 = e_0 + p_0 v_0 + D^2/2 \equiv \mathcal{H} \tag{3}$$

The constants of the right hand sides of the last expressions are evaluated in the ambient mixture. For the ideal equation of state one has $e + pv = c^2/(\gamma - 1) - Q\lambda$. The algebraic relations are the Rankine–Hugoniot conditions that hold at the shock and at each point in the structure as λ changes from 0 at the shock to 1 at complete reaction.

It is straightforward to eliminate pressure and velocity in favor of specific volume to write a single algebraic equation for v for a given value of D. In the case of the ideal equation of state, this equation is a quadratic and has two solutions available. The character of this algebra is apparent by an alternative, graphical solution procedure that uses the mass relation to substitute for the velocity in the momentum equation to obtain a linear relation (known as the Rayleigh or Michelson–Rayleigh line) beween p and v in a p, v plane. And in a similar way, one substitutes for U in the energy equation to obtain a relation between p and v, known as the Hugoniot curve (which for the ideal equation of state is a hyperbola). Because both relations depend on D for a fixed Q, there is a minimum value of D such that this algebra allows a structure that starts at the shock state (with $\lambda = 0$) and terminates at the complete reaction state (at $\lambda = 1$). Specifically, the minimum value of D has the Rayleigh line tangent to the complete reaction Hugoniot curve. For the ideal equation of state, the minimum velocity is found by setting $\lambda = 1$ and setting the discriminant of the quadratic equal to zero, which leads to the simple formula for D_{CJ},

$$D_{CJ} = \sqrt{q} + \sqrt{c_0^2 + q}, \quad \text{where } q = Q(\gamma^2 - 1)/2 \tag{4}$$

The solution for v is expressed simply as [87]

$$\frac{v}{v_0} = \frac{\gamma}{\gamma + 1} \frac{(c_0^2/\gamma + D_n^2)}{D_n^2}(1 - \delta) \tag{5}$$

where δ^2 is given by

$$\delta^2 = b^2(1 + F - \lambda) \tag{6}$$

with

$$b = \frac{(D_{CJ}^2 - c_0^2)}{(c_0^2 + \gamma D_n^2)} \frac{D_n}{D_{CJ}}, \qquad F = (D_n^2 - D_{CJ}^2) \frac{D_n^2 D_{CJ}^2 - c_0^4}{D_n^2 (D_{CJ}^2 - c_0^2)^2} \tag{7}$$

The velocity and pressure are found from successive substitutions to obtain

$$U = \mathcal{M} v, \qquad p = \mathcal{P} - \mathcal{M}^2 v \tag{8}$$

If we introduce the local normal Mach number (squared) in the shock-attached frame, $\mathsf{M}^2 = U^2/c^2$, then simple algebra shows that δ^2 can also be rewritten compactly as

$$\delta^2 = \left(\frac{1 - \mathsf{M}^2}{1 + \gamma \mathsf{M}^2} \right)^2 \tag{9}$$

Importantly, this equation illustrates that the argument of the square root that defines δ is always positive. If $D > D_{CJ}$, then the detonation is overdriven and $F > 0$; if $D = D_{CJ}$, then $F = 0$ and the steady CJ state is obtained with $\mathsf{M} = 1$, that is, $U = -c$, and therefore $\delta = 0$.

The spatial distribution of reactants in a steady detonation $\lambda(n)$ is calculated by integrating the rate equation,

$$n(\lambda) = \int_0^\lambda \frac{U \, d\bar{\lambda}}{\omega} \tag{10}$$

The steady half-reaction length $\ell_{1/2}$ is defined for a specified values of $D \geq D_{CJ}$ as the distance measured from the shock to a point in the reaction zone where the reaction progress variable is $\frac{1}{2}$, that is, $\ell_{1/2} = \int_0^{1/2} (U d\bar{\lambda})/\omega$. First introduced by Erpenbeck, this length is often used as the length scale for dimensional analysis. It is straightforward to generate the extension of these results to a general equation of state and rate law for a single progress variable, albeit there is no general analytic expression that corresponds to (10), and a numerical root finding procedure must be used to compute the structure for the general case.

D. Stability Formulation

The first step is to transform the equations to the shock-attached coordinate frame as shown in Fig. 2. Again, let n be a coordinate parallel to the x axis that in turn is in the direction of a planar steady propagation of detonation traveling at speed D, so that the coordinate transformation is given by

$$n = x - Dt - \psi(y, t) \tag{11}$$

Then various differential operators in the governing equations transform as follows:

$$\frac{\partial}{\partial t} \to \frac{\partial}{\partial t} - \left(D + \frac{\partial \psi}{\partial t}\right)\frac{\partial}{\partial n}, \qquad \frac{\partial}{\partial x} \to \frac{\partial}{\partial n}, \qquad \frac{\partial}{\partial y} \to \frac{\partial}{\partial y} - \frac{\partial \psi}{\partial y}\frac{\partial}{\partial n} \tag{12}$$

In this shock-attached frame the governing equations can be written in a matrix form,

$$\frac{\partial \boldsymbol{q}}{\partial t} + \boldsymbol{A}_n \cdot \frac{\partial \boldsymbol{q}}{\partial n} + \boldsymbol{A}_y \cdot \frac{\partial \boldsymbol{q}}{\partial y} - \boldsymbol{B}_y \cdot \frac{\partial \boldsymbol{q}}{\partial n}\frac{\partial \psi}{\partial y} + \boldsymbol{a}\frac{\partial^2 \psi}{\partial t \partial y} + \boldsymbol{b}\frac{\partial^2 \psi}{\partial t^2} = \boldsymbol{c} \tag{13}$$

where $\boldsymbol{q} = (v, U_1, u_2, p, \lambda)^T$ is the state vector in which the particle velocity is defined in the frame of the perturbed shock, that is $U_1 = u_1 - D - \partial\psi/\partial t$, and the transverse component u_2 is the same as in the laboratory frame. The rest of the matrices and column vectors are listed in the Appendix. Linear stability theory deals with solutions of (13) that deviate by a small amount from some steady-state solution. One makes a small amplitude expansion about the steady state, of the form

$$\boldsymbol{q} = \boldsymbol{q}^* + \epsilon \boldsymbol{q}'(n)\exp(\alpha t + iky), \qquad \psi = \epsilon\psi'\exp(\alpha t + iky) \tag{14}$$

Here the base steady-state is $\boldsymbol{q}^* = (v^*, U^*, 0, p^*, \lambda^*)^T$, the perturbation-amplitude vector is $\boldsymbol{q}' = (v', u_1', u_2', p', \lambda')^T$, and ϵ is the disturbance-amplitude norm. The normal-mode expansion seeks for a restricted class of asymptotic solutions to the general small amplitude initial-value problem, which leads to sufficient conditions for instability. Because solutions to a homogenous system are sought, we can set the shock amplitude $\psi' = 1$ as its dimensional value is a common factor in the resulting homogeneous relations.

Derivation of the linear equation for $\boldsymbol{q}'$ is straightforward and results in the following homogeneous linear system for the perturbation amplitudes,

$$\boldsymbol{A}^* \cdot \frac{\mathrm{d}\boldsymbol{q}'}{\mathrm{d}n} + (\alpha \boldsymbol{I} + \boldsymbol{C}^*) \cdot \boldsymbol{q}' + \boldsymbol{b}^* = 0 \tag{15}$$

The matrices $\boldsymbol{A}^*$, $\boldsymbol{C}^*$, and the vector $\boldsymbol{b}^*$ are functions of the steady-state solution, the sought-for growth rate α and the wave number k, and are given by

$$\boldsymbol{A}^* = \begin{bmatrix} U & -v & 0 & 0 & 0 \\ 0 & U & 0 & v & 0 \\ 0 & 0 & U & 0 & 0 \\ 0 & \rho c^2 & 0 & U & 0 \\ 0 & 0 & 0 & 0 & U \end{bmatrix}^*, \qquad \boldsymbol{b}^* = \begin{bmatrix} 0 \\ \alpha^2 \\ -ikv\,\mathrm{d}p/\mathrm{d}n \\ 0 \\ 0 \end{bmatrix}^* \tag{16}$$

$$\boldsymbol{C}^* = \begin{bmatrix} -\mathrm{d}U/\mathrm{d}n & \mathrm{d}v/\mathrm{d}n & -ikv & 0 & 0 \\ \mathrm{d}p/\mathrm{d}n & \mathrm{d}U/\mathrm{d}n & 0 & 0 & 0 \\ 0 & 0 & 0 & ikv & 0 \\ (\gamma-1)Q\rho(\rho\omega - \omega_v) & \mathrm{d}p/\mathrm{d}n & ik\rho c^2 & \gamma\mathrm{d}U/\mathrm{d}n - (\gamma-1)Q\rho\omega_p & -(\gamma-1)Q\rho\omega_\lambda \\ -\omega_v & \mathrm{d}\lambda/\mathrm{d}n & 0 & -\omega_p & -\omega_\lambda \end{bmatrix}^* \tag{17}$$

Here ω_p, ω_v, and ω_λ are the reaction rate sensitivities as obtained by the expansion of the reaction rate law as $\omega' = \omega_v^* v' + \omega_p^* p' + \omega_\lambda^* \lambda'$, where the subscripts in ω denote partial differentiation. Linearization of the shock relations leads to conditions on perturbations that must be satisfied at the shock, $n = 0$, at all times,

$$p' = \frac{4\rho_0 D}{\gamma+1}\alpha, \qquad v' = -\frac{4c_0^2}{(\gamma+1)\rho_0 D^3}\alpha \tag{18}$$

$$u_1' = \frac{2c_0^2 - (\gamma-1)D^2}{(\gamma+1)D^2}\alpha, \qquad u_2' = \frac{2(c_0^2 - D^2)}{(\gamma+1)D}ik, \qquad \lambda' = 0 \tag{19}$$

E. Radiation (Closure) Condition

The radiation condition is a closure condition that is applied at the end of the reaction zone of the steady wave. It can be interpreted as a condition that the perturbations are spatially uniform (i.e., do not blow up) in the steady reaction zone. This was the original interpretation given by Erpenbeck and is the one consistent with developing a uniform asymptotic solution of the initial-value problem, where the disturbance amplitude is initially prescribed as uniformly $\mathcal{O}(\epsilon)$. If the reaction rate kinetics is such that the steady reaction zone terminates at infinity, then the radiation condition is interpreted properly as a causality condition. In the far field one has a near constant state with attendant linear acoustics to leading order. In this case the radiation condition is simply derived by decomposing the linear acoustics into families of waves that travel at the real characteristic speeds and insisting that the solution there does not depend on the wave family that points toward the shock. This means that the flow disturbances in the far field do not influence the evolution of the reaction zone. Literally, it means that the solution depends on a superposition of waves that are degenerate in the sense that one wave family is absent. For a linear disturbance this means that the perturbations of the state variables must be related by a simple linear combination of the perturbed variables.

If one assumes that the state at the tail of the reaction zone is a constant state to first order then all steady-state gradients are zero. In this region we will use the laboratory frame x component of velocity instead of the shock frame and in $\boldsymbol{q}'$ replace u_1' with $u' - \partial\psi'/\partial t$, hence $\boldsymbol{b}^*$ is absorbed into the redefinition of $\boldsymbol{q}'$ and the shock acceleration does not appear as a forcing term in the acoustic equations. In what follows, the ∞ subscript is implied unless stated otherwise and is added for clarification if needed. For the convenience of the analysis we will assume that the spatial dependence on n is represented as a Fourier mode $\boldsymbol{q}' = \hat{\boldsymbol{q}}\exp(i\sigma n)$, so that linear stability equations reduce to

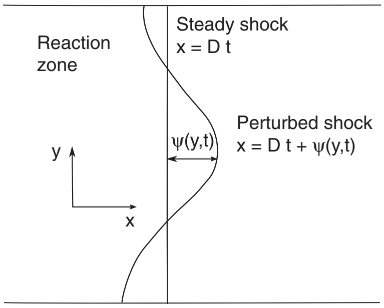

Fig. 2 Schematics of the shock-attached frame for 2-D detonation.

$$(\alpha \boldsymbol{I} + i\sigma \boldsymbol{A}^* + \boldsymbol{C}^*)_\infty \hat{\boldsymbol{q}} = 0 \tag{20}$$

with

$$(\alpha \boldsymbol{I} + i\sigma \boldsymbol{A}^* + \boldsymbol{C}^*)_\infty = \begin{bmatrix} \alpha + i\sigma U & -i\sigma v & -ikv & 0 & 0 \\ 0 & \alpha + i\sigma U & 0 & i\sigma v & 0 \\ 0 & 0 & \alpha + i\sigma U & ikv & 0 \\ 0 & i\sigma\rho c^2 & ik\rho c^2 & \alpha + i\sigma U & -(\gamma-1)Q\rho\omega_\lambda \\ 0 & 0 & 0 & 0 & \alpha + i\sigma U - \omega_\lambda \end{bmatrix} \tag{21}$$

The dispersion relation is found be setting $\det(\alpha \boldsymbol{I} + i\sigma \boldsymbol{A}^* + \boldsymbol{C}^*)_\infty = 0$ to obtain

$$(\alpha + i\sigma U)^2(\alpha + i\sigma U - \omega_\lambda)[(\alpha + i\sigma U)^2 + c^2(k^2 + \sigma^2)] = 0 \tag{22}$$

For fixed α there are five possible values for σ with a double root given by

$$\sigma_{1,2} = i\alpha/U_\infty \tag{23}$$

that corresponds to vorticity and entropic waves, two roots,

$$\sigma_{3,4} = \frac{-i\alpha U \pm ic\sqrt{\alpha^2 + k^2(c^2 - U^2)}}{c^2 - U^2} \tag{24}$$

that correspond to acoustic waves, and one root,

$$\sigma_5 = i\left[\alpha - \frac{(\omega_\lambda)_\infty}{U_\infty}\right] \tag{25}$$

that is associated with residual chemical reaction.

There are five eigenvectors (written as column vectors) associated with these roots and from these one can construct the matrix $\boldsymbol{R} = [\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3, \boldsymbol{r}_4, \boldsymbol{r}_5]$ with the eigenvectors in the columns:

$$\boldsymbol{R} = \begin{bmatrix} 1 & 0 & -\frac{1}{\rho c^2} & -\frac{1}{\rho c^2} & \frac{\sigma_5^2 + k^2}{\rho^2\omega_\lambda^2} \\ 0 & 1 & -\frac{iv\sigma_3}{\alpha + i\sigma_3 U} & -\frac{iv\sigma_4}{\alpha + i\sigma_4 U} & -\frac{i\sigma_5}{\rho\omega_\lambda} \\ 0 & -\frac{\sigma_2}{k} & -\frac{ivk}{\alpha + i\sigma_3 U} & -\frac{ikv}{\alpha + i\sigma_4 U} & -\frac{ik}{\rho\omega_\lambda} \\ 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & \frac{c^2\left(\sigma_5^2 + k^2\right) + \omega_\lambda^2}{(\gamma-1)Q\rho\omega_\lambda^2} \end{bmatrix} \tag{26}$$

Then one can write a general disturbance as

$$\boldsymbol{q}' = \boldsymbol{R}\boldsymbol{c} \tag{27}$$

with $\boldsymbol{c}$ being a vector of coefficients that multiply the linearly independent solutions $\boldsymbol{r}_i$. One solves for $\boldsymbol{c}$ as

$$\boldsymbol{c} = \boldsymbol{R}^{-1}\boldsymbol{q}' \tag{28}$$

and the radiation condition is found by suppressing the incoming wave $\boldsymbol{r}_4$ associated with the C_+ (i.e., the $u + c$) characteristic, which is associated with σ_4. Hence the compatibility condition is found by setting $c_4 = 0$. This in turn is a scalar homogeneous linear relation between the components of $\boldsymbol{q}'$, which is represented as

$$\frac{i\alpha u'}{U} + kv' - i\frac{vp'}{Uc}\sqrt{\alpha^2 + k^2(c^2 - U^2)} + i\lambda'\omega_\lambda\frac{(\gamma-1)Q}{c^2} \times \left[\frac{(\alpha^2 - U^2k^2) - \omega_\lambda[\alpha + (U/c)\sqrt{\alpha^2 + k^2(c^2 - U^2)}]}{[(\alpha - \omega_\lambda)^2 - k^2U^2] - (U^2/c^2)\omega_\lambda^2}\right] = 0 \tag{29}$$

In many problems of interest, the reaction rate is highly state sensitive and the rate at the end of the reaction zone is much smaller than at the shock and throughout the bulk of the steady-state reaction zone. This is typically the case when the reaction rate is of Arrhenius form and the rate is exponentially small at the end of the reaction zone in comparison to elsewhere. Then one can show that the perturbations of λ decay rapidly toward the end of the reaction zone and can be neglected so that the radiation condition simplifies to

$$\frac{i\alpha u'}{U} + kv' - i\frac{vp'}{Uc}\sqrt{\alpha^2 + k^2(c^2 - U^2)} = 0 \tag{30}$$

In many cases there is no appreciable difference in the computed dispersion relations.

F. Numerical Solution and Techniques

The problem that determines the dispersion relation governing linear disturbances $\boldsymbol{q}'$ is given by (15), and $\boldsymbol{q}'$ satisfy the shock relations (18) and the radiation condition (29). The normal-mode representation assumes that $\boldsymbol{q}'$ and α are complex (whereas k is real) and hence, counting the real and imaginary parts, ten ordinary differential equations are subject to ten shock conditions and two radiation conditions. Because the shock conditions provide boundary conditions to entirely determine the solution in terms of given parameters and α and k, the two extra conditions afforded by the radiation condition can be thought of as conditions that determine the real and imaginary parts of α. The problem thus formulated is entirely general and can be solved by any means, analytical or numerical.

Because the coefficients of the governing ODEs are not constant, numerical solution provides the simplest means for comprehensive exploration of the parameters. A robust and simple-to-implement numerical (shooting) method for this problem was first introduced in [36]. To devise a solution procedure, a numerical integration package to integrate a system of ODEs (preferably one that can handle stiff ODEs) and a numerical root finding package are required. One assumes fixed values for all physical parameters, for example, Q, γ, growth rate α, and wave number k, except for two. Those two can in principle be any two in the previous list. Then one assigns trial values for those remaining two values. Subsequently, all the values are defined so that one can integrate from the shock at $n = 0$ to a remote point $n = -L$ in the steady reaction zone. Then one tests whether the radiation condition is satisfied by computing the residual defined by (29). The residuals can then be used to derive new seed guesses for the next iteration. In some cases, one can use the steady reaction progress variable $\lambda^*(n)$ and replace dependence on n by dependence on λ^*. This requires a straightforward coordinate transformation of the governing equations and then one integrates from the shock at $\lambda^* = 0$ to a remote point in the steady reaction zone $\lambda^* = 1 - 1/N$, where N can be used simultaneously to control the resolution of the integration of the steady domain and the distance to the remote point. The advantage of this strategy is that only one integration parameter is required.

The core procedure described above can be used to find individual values of the growth rate α or any other pair of parameters with the rest of the parameters fixed. In particular, one can use automated continuation methods to find neutral stability curves for modal branches. One sets $Re(\alpha) = 0$, sets all the other parameters save one undetermined, like the heat of detonation Q (say), and iterates on $Im(\alpha)$ and that parameter, (such as Q). Entire branches can be found in single runs. The global neutral stability curve is of course found by composition of all of the modal branches.

Because the method is essentially a root finding procedure, seed values for the two sought-after values are required. For fixed physical parameters, one can rapidly generate a map of approximation of the locations of the growth rate α in the complex plane by partitioning the plane into a section, and evaluating the complex residual defined by (29) at each point in the partition. One then generates a contour map of some norm (like the square root of the sum of the squares) of the complex residual. The resulting map, at sufficiently dense resolution for the section of the plane, will clearly show closed contours that indicate the possible location of the sought-after roots. Local searches or traverses can be carried out to find the roots. The procedure can be automated with a minimum of programming complexity. A detailed description of the methodology can be found in [36].

G. Example for the Basic Model

In this section we give a sample calculation of the instability spectrum using the methodology described above. We choose the following parameters: $\gamma = 1.222$, $Q = 45.2$, $E = 52.5$, and $f = 1.6$, which are representative of the stoichiometric hydrogen–air mixture. In an oblique detonation, the overdrive factor is determined by the wedge angle at a given inflow Mach number or by the Mach number for a given wedge angle. By controlling either one of the two parameters, one can vary the overdrive factor in a wide range and thus control the instability. Indeed, generally, detonations become more stable as the overdrive factor is increased. We choose $f = 1.6$ so that the corresponding two-dimensional planar detonation has only a few unstable modes; this overdrive is also representative of real experiments. If f is too large, then detonation will be stable, whereas as f tends to unity, the number of unstable modes grows and can be quite large.

We also note here that if one considers a free oblique detonation wave (i.e., no wedge or any other boundary present), then a simple coordinate transformation to a frame moving along the oblique shock with velocity equal to the tangential component of the incoming velocity, reduces the linear stability problem for the oblique detonation to that of a planar detonation, in which the detonation speed is equal to the normal component of the incoming flow. Such a coordinate transformation has no effect on the growth rate of unstable modes and hence on the neutral stability boundary, but the frequency will be affected by a term proportional to the frame velocity. Thus the instability of a free oblique detonation is governed by the same mechanisms as that of a planar detonation.

A significant physical consequence of having an oblique detonation on a wedge is that perturbations, even if unstable, may not necessarily affect the wave in the region of interest, because the perturbations will be convected along the front and locally may even appear as stable. Thus one must be careful to distinguish absolute and convective instabilities of the oblique detonation.

When attempting to model a real gaseous mixture with a single-step reaction one is always faced with a choice of representative parameters. The simplified model attempts to describe the complex real mixture with γ, E, Q specified. One obviously cannot expect too much from such a simplified model, yet it does provide much valuable detailed information that is quite relevant to realistic detonations at least on a qualitative level. Our choice of parameters here follows the same guidelines as in [87], that is we choose the parameters so that the activation energy and the heat of reaction are the same as those fitted to the one-dimensional numerical calculations using detailed chemistry [89], and the specific-heat ratio is determined from Rankine–Hugoniot conditions by demanding

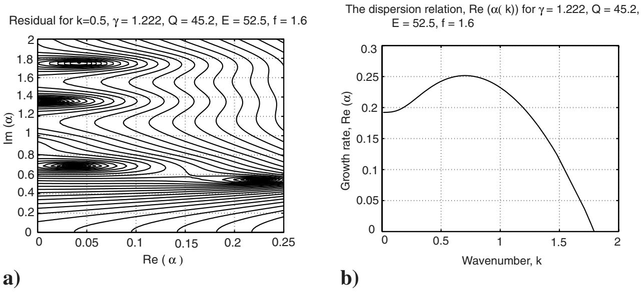

Fig. 3 a) Contour plot of the residual function showing the location of the eigenvalues at $k = 0.5$. b) The growth rate vs wave number for the most unstable fundamental mode.

that the simplified model predict the von Neumann temperature in agreement with detailed calculations. This choice of parameters retains from reality what is most essential: overall energetics, the strength of the rate dependence, and the state sensitivity at the shock, where the reaction just begins.

Because all calculations below are done in dimensionless units of half-reaction length and half-reaction time, it is useful to know the characteristic length of the reaction zone, which in our case is $l_{rz} = 0.215$ mm. The corresponding time scale is $t_{rz} = l_{rz}/c_s$, where c_s is the postshock sound speed ($c_s = 3.075$ in units of $\sqrt{p_0 v_0}$). One can easily find dimensional quantities of interest, if desired.

Figure 3a shows a typical contour plot of the magnitude of the radiation condition (30) in which one can see approximate locations of the eigenvalues. The contour plots provide a necessary initial guess for subsequent accurate calculations of the roots. The fundamental lowest frequency root is seen to have much larger real part than the rest of the spectrum. In fact, in this particular case, the fundamental mode has a global maximum for all k, as shown in Fig. 3b, at $k = 0.7$, $\alpha = 0.252 + i0.669$. The higher harmonics, unstable at larger k when the fundamental mode stabilizes, have growth rates much smaller than the global maximum, and at even larger k they also appear to stabilize.

The present calculation is included as a typical result of a linear stability calculation and is not intended for direct comparisons with either physical experiment or numerical simulation of the oblique detonation on a wedge. There are several issues that to a large degree would invalidate such comparisons. The most obvious one is that the analysis is linear and thus is unable to predict the prominent nonlinear features of observed detonations. One must also keep in mind that the linear analysis along the lines described in this paper is limited to unconfined detonations (except [49]), but the wedge-stabilized detonation is intrinsically coupled to the wedge boundary and is likely to be strongly affected by the wave interactions with the boundary. Hence a completely different analysis is required for adequate comparisons. To complicate the matter further, the underlying steady detonation, whose stability is meant to be explored by the linear stability theory, is two dimensional, hence the linearized system does not easily reduce to a system of ordinary differential equations.

In view of these difficulties, we think there is a necessity for high-accuracy numerical algorithms for multidimensional detonation simulations if any significant advance is to be made. It is appropriate to mention here a recent numerical work [75] in which the authors developed a highly accurate method to simulate one-dimensional detonations using coordinate transformation attached to the lead shock [74]. Extensions of such techniques to multidimensional problems would be invaluable not only in simulations of practical value but also in helping to reconcile available theoretical work with numerical experiments.

IV. Conclusions

Multidimensional, time-dependent simulation is likely to be the principal tool for investigating the nonlinear stability of detonation flows related to propulsion. Theory can be invaluable in verifying the underlying computational accuracy of such codes and also is of vital importance to basic understanding. For the purposes of actual design, direct comparison with experiment should be an essential part of any new theoretical developments. The reason for this is because detonations are generally so unstable, multiscale, and often exponentially state dependent, that it is very easy to develop theories that are far removed from applications, and while interesting, are not terribly useful except in the most general ways.

It is striking that for the very simple configuration of a premixed detonable inlet flow anchored by a wedge, there is no well-established analytical theory. Also there are only a handful of reports of useful simulations in the literature. It would be reasonable to establish a set of parameters that might correspond to the operational states of a real engine in a flight cycle or similar combustion experiment, and explore all the dynamic states of that detonation flow to see if there indeed is a true operational window where the detonation would be stabilized and robust. Such a program should also be carried out with concurrent experiment or access to experiment. Certainly, it would be worthwhile to carry out more high quality simulations in both the wedge and blunt body configurations because these are accessible by theory, simulation, and experiment. This is a very large undertaking given the size of the needed computations. Continued improvement in algorithms and the efficient use of large computing resources are essential to success.

For stabilized steady or cyclically steady detonation flows, it is likely that the issue of sonic self-confinement is very important and is a central theoretical consideration. Just like our example of a solid rocket motor with a sonic disk at the throat, in any detonation configuration envisioned that is stable and long-lived, there is likely to be a causal domain that includes the lead shock, reflected shocks, and wall confinement that form the boundaries of the domain of dependence, which also includes the sonic locus. Understanding the properties of the multidimensional characteristic surfaces is likely to lead to a much greater understanding of mechanisms of the detonation process and its nonlinear stability than what we know now.

The asymptotic theories that predict cellular detonations, such as those due to Yao and Stewart [61], Clavin and Denet [70], need to be reconciled, albeit they are in very different limits (near CJ and highly overdriven, respectively). Likewise, the weakly nonlinear stability theory for overdriven detonation described by Bourlioux, Majda, and Roytburd [37,42,76] has not led to a demonstration of cells, and that aspect of the theory should be regarded as incomplete. For long-lived stable detonation cell complexes with long wavelength features but persistent high-frequency cells, one would assume that one can average over the high wave numbers and generate a reduced long wavelength theory for the lead shock dynamics that has terms that represent the contributions from the high-frequency cells. Such a theory, if matched to experiment and validated, might be invaluable for engineering design.

Appendix: Definition of Matrices

$$\boldsymbol{A}_\eta = \begin{bmatrix} U & -v & 0 & 0 & 0 \\ 0 & U & 0 & v & 0 \\ 0 & 0 & U & 0 & 0 \\ 0 & \rho c^2 & 0 & U & 0 \\ 0 & 0 & 0 & 0 & U \end{bmatrix} \qquad \boldsymbol{A}_y = \begin{bmatrix} u_2 & 0 & -v & 0 & 0 \\ 0 & u_2 & 0 & 0 & 0 \\ 0 & 0 & u_2 & 0 & 0 \\ 0 & 0 & 0 & u_2 & 0 \\ 0 & 0 & 0 & 0 & u_2 \end{bmatrix} \tag{A1}$$

$$\boldsymbol{B}_y \cdot \boldsymbol{q}_n = \begin{bmatrix} u_2 \frac{\partial v}{\partial n} - v \frac{\partial u_2}{\partial n} \\ u_2 \frac{\partial U}{\partial n} \\ u_2 \frac{\partial u_2}{\partial n} + v \frac{\partial p}{\partial n} \\ u_2 \frac{\partial p}{\partial n} + \rho c^2 \frac{\partial u_2}{\partial n} \\ u_2 \frac{\partial \lambda}{\partial n} \end{bmatrix}, \qquad \boldsymbol{a} = \begin{bmatrix} 0 \\ u_2 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \qquad \boldsymbol{b} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}$$
$$\boldsymbol{c} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \rho c^2 \sigma \omega \\ \omega \end{bmatrix} \tag{A2}$$

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