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Overturning of nonlinear acoustic waves. Part 1 A general method

By P. W. HAMMERTON AND D. G. CRIGHTON

Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Silver Street, Cambridge CB3 9EW, UK

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We consider model nonlinear wave equations of the form $u_t + uu_x = \mathscr{H}(x, t; u, u_x, \ldots)$ arising in gasdynamics and other fields, $\mathscr{H}$ incorporating various linear mechanisms of dissipation and dispersion. If $\mathscr{H}$ includes a thermoviscous dissipation term ϵu_{xx}, then it is generally believed that $u(x, t)$ will remain single-valued for all $t > 0$ and all single-valued $u(x, 0)$, for any $\epsilon > 0$. The question addressed here is whether, if thermoviscous dissipation is excluded from $\mathscr{H}$, $u(x, t)$ remains single-valued for all $t > 0$, or whether certain dissipative–dispersive mechanisms (such as relaxation processes) are in themselves insufficient to prevent wave overturning. To answer this we propose a numerical scheme based on the use of intrinsic coordinates $\psi = \psi(s, t)$ to describe the waveform at each time. In this paper, the method is described and validated by comparisons with the exact solutions for certain $\mathscr{H}$ ($\mathscr{H} = 0$, $\mathscr{H} = -\alpha u$, $\mathscr{H} = \epsilon u_{xx}$). These comparisons show that the scheme is free of numerical viscosity effects which preclude the solution of the problem by finite-difference or spectral methods applied to the signal $u(x, t)$, that it can reliably distinguish between finite-time overturning and merely the formation of steep gradients, and that it can accurately predict the time of overturning when it does occur. Having established the validity of the method, attention can then be turned to those cases where criteria for overturning have not as yet been determined by conventional methods. In Part 2, harmonic wave propagation through a relaxing gas is investigated.

1. Introduction

In the standard linear theory of sound, waves propagate with constant energy and uniform wave speed. However, the finite amplitude of the signal gives rise to nonlinear effects which, though weak, act cumulatively and thus may become significant over long ranges. Compressive phases of a disturbance travel faster than expansive phases and hence wave crests tend to catch up with wave troughs, with the result that steepening of the wave occurs. This wave steepening increases the importance of other physical processes; the local increase in wave slope means that attenuation or dispersion effects that can be ignored for small wave slopes may ultimately become significant. If such effects are ignored entirely in the nonlinear theory, wave steepening will eventually lead to the wave 'breaking', with multi-valued solutions of the wave equation being obtained. Although the concept of wave breaking or overturning is meaningful only in certain physical situations, such as surface water waves, we use these terms synonymously with the onset of multi-valued solutions. In the context of acoustic propagation, the actual overturning of waves is clearly physically meaningless, pointing instead to a deficiency in the model equation. This paper is concerned with

investigating the way in which different physical mechanisms act to inhibit wave overturning.

For acoustic propagation through a real medium, where many competing physical effects may be present, it becomes important to identify which mechanisms are of fundamental importance in determining the shape of the waveform. Straightforward comparison of the initial magnitudes of the various physical mechanisms leads to a set of dimensionless parameters, such as the inverse acoustic Reynolds number which expresses the relative magnitudes of the thermoviscous diffusivity and the nonlinearity. These parameters characterize the nominal relative importance of the different physical effects, at least before significant wave steepening occurs, and may also suggest a scaling for any narrow shock-type region which may arise. However, a more detailed analysis is then necessary in order to determine which mechanisms are ultimately significant. Thus we envisage a situation where one linear mechanism initially dominates all others, and then ask whether the same physical effect remains dominant over the whole profile at much greater propagation ranges. For this reason, we examine the effect of various such mechanisms in isolation, and consider whether or not physically realizable solutions are obtained; that is, is wave steepening sufficiently impeded for wave overturning to be prevented?

In §2, we give model equations which include various physical effects. Attention is restricted to the case of plane wave propagation, in which case the equations can all be written in the form

$$u_t + uu_x = \mathscr{H}(x, t; u, u_x, \ldots), \tag{1.1}$$

where $\mathscr{H}(x, t; u, u_x, \ldots)$ represents a particular linear attenuation and dispersion mechanism. As usual, quasi-plane waves (for example, diverging cylindrical or spherical waves far from the source) may be included in the class (1.1) through appropriate transformations of the dependent and independent variables. Thermoviscous diffusion is believed always to produce only single-valued solutions, but for other physical mechanisms, the situation is much less clear-cut, and may depend crucially on the relative magnitudes of certain parameters. For propagation through a relaxing medium, we demonstrate in Part 2 (Hammerton & Crighton 1993) that the existence of physically meaningful solutions, in the absence of diffusivity, depends on the characteristic scales of the initial disturbance and on the material parameters of the medium.

If the nominal magnitude of the linear mechanism $\mathscr{H}$ is small in comparison with that of the nonlinearity, analytical progress can be made by the method of matched asymptotic expansions (Crighton & Scott 1979). Essentially, the argument is that the lossless solution is obtained by the method of characteristics. Then in the vicinity of any spatial region containing large gradients, where the ignored attenuation or dispersion terms will have become significant, new scalings are introduced and it is then considered as a 'transition region' in which the solution changes rapidly, but continuously, between two values. Accordingly, the presence of single- or multi-valued solutions *for such a transition region* is the only thing that needs to be investigated. If attention can be restricted to travelling wave solutions for this transition, as is commonly the case, the problem becomes more amenable to analytic investigation and it may be possible to establish a criterion for the existence of single-valued travelling wave solutions as a function of the dimensionless parameters and the transition amplitude. In this way, using the local transition or 'shock' analysis and the lossless outer solutions, conditions for which multi-valued solutions arise can be obtained. However, if attenuation and dispersion effects become generally comparable with the effect of nonlinearity over the whole wave, it is clear that this approach breaks down.

In the absence of exact solutions, progress can then only be made using arguments based on functional analysis, or by numerical investigations. The first approach is taken by Naumkin & Shishmarev (1982, 1983) who consider the phenomenon of wave breaking for disturbances governed by Whitham's equation (Whitham 1967) in which the dissipation and dispersion effects are modelled by a general linear convolution integral term. Sufficient conditions for the appearance of multi-valued solutions are determined, but determination of the necessary criterion is unattainable. On the other hand, direct numerical solution of the model equations can never properly determine the appearance of multi-valued solutions because of diffusive effects inherent in numerical schemes. This paper is concerned with reformulating the physical equation, for a general linear mechanism, in such a way that numerical investigation of wave overturning becomes possible.

In order to investigate overturning by numerical means, a very different approach must be taken to solving the nonlinear wave equation. Clearly, it is vital to distinguish between $\partial u/\partial x$ becoming infinite in finite time (i.e. the appearance of a multi-valued solution and wave overturning) and $\partial u/\partial x$ becoming very large but remaining finite (as in the case of Burgers' equation with a small coefficient of diffusivity). Direct solution of the physical equation by the usual finite-difference or spectral schemes can never reveal this difference. As the maximum gradient increases, more and more mesh points must be included to retain resolution, but even so, true identification of overturning can never be accomplished. In addition, many such numerical schemes inherently introduce a small amount of numerical viscosity which limits the growth of gradients, so predicting single-valued solutions in all cases. The governing equation must therefore be re-expressed in a form which eliminates the singularity caused by infinite spatial gradients. A natural way to tackle this is to recast the governing equations into characteristic form. For some of the model equations introduced in §2 this reformulation proves to be straightforward, but in other cases the problem become much more difficult, if not impossible. It is for this reason that we focus attention on finding a general method which is applicable to a large class of equations.

In this paper, what is believed to be a new method of describing wave overturning is introduced. By expressing the wave profile in terms of *intrinsic coordinates*, to be defined in due course, all the difficulties associated with the onset of wave overturning are circumvented and accurate times for wave breaking can be obtained. In addition, use of this method allows the wave profile to be accurately determined, and easily visualized, at all points of its evolution. The details of this intrinsic coordinate formulation are given in §3. It appears that analytical progress using this formulation is limited, so in §4 the numerical implementation of the method is discussed. In cases where exact solutions are available, comparison is made between such solutions and the numerical results and found to be extremely favourable. In Part 2, the intrinsic coordinate approach is used to investigate nonlinear propagation through relaxing media.

2. Model equations

A wide range of model equations describing weakly nonlinear acoustic propagation through various media is available (see, for example, Crighton 1979). In all the cases considered here, the origins of the nonlinearity are the same, namely the convective terms in the fluid mass and momentum conservation equations, and the local nonlinearity of the pressure–density relation. Thus the nonlinearity always appears in the same way in the equations discussed below and it is the inclusion of different *linear*

mechanisms that gives rise to radically different propagation behaviour. The essential nonlinearity for uni-directional flow is represented in the simple (Riemann) wave equation

$$U_T + [a_0 + \tfrac{1}{2}(\gamma+1)\,U]\,U_X = 0, \tag{2.1}$$

where U is the disturbance fluid velocity, X the space coordinate, T the time, a_0 the small-signal sound speed and γ the adiabatic exponent or an equivalent parameter for a condensed fluid. In order to make the analysis of §§3 and 4 algebraically clearer, the equations to be studied are considered in non-dimensional form with respect to a steadily moving frame. Thus (2.1) is written in the form

$$u_t + uu_x = 0, \tag{2.2}$$

where $x \propto X - a_0 T$ and $t \propto T$.

Inclusion of thermoviscous diffusion leads to the familiar Burgers equation (Lighthill 1956)

$$u_t + uu_x = \Delta u_{xx}, \tag{2.3}$$

where Δ is the non-dimensional diffusivity of sound. Varley & Rogers (1969), on the other hand, included viscoelastic damping effects and obtained the model equation

$$u_t + uu_x = -\alpha u. \tag{2.4}$$

For propagation of waves through a gas-filled pipe, the cumulative effect of wall friction in the Stokes boundary layer(s) leads to

$$u_t + uu_x = \beta \int_0^\infty \frac{u_x(x, t-\xi)}{\xi^{\frac{1}{2}}}\,\mathrm{d}\xi \tag{2.5}$$

(Chester 1964), which can be regarded as saying that the wall effect gives rise to a fractional derivative (Sugimoto 1989, 1991).

In many real gases, internal thermodynamic variables of state do not respond immediately to changes in conditions caused by a disturbance such as a sound wave and so *relaxation* effects may become significant. If a single relaxation time characterizes the non-equilibrium variable, the equation for uni-directional propagation (Polyakova, Soluyan & Khokhlov 1962; Blythe 1969; Ockendon & Spence 1969) can be written in the non-dimensional form

$$u_t + uu_x = -\frac{\Gamma}{\Omega} \mathrm{e}^{x/\Omega} \int^x \mathrm{e}^{-x'/\Omega} u_{x'x'}\,\mathrm{d}x', \tag{2.6}$$

where Ω is proportional to the relaxation time, and Γ is proportional to the difference between high-frequency (frozen) and zero-frequency (equilibrium) sound speeds. The theory underlying this equation is briefly discussed in Part 2, which is devoted to nonlinear propagation through such relaxing gases.

It can thus be seen that many of the equations of interest in nonlinear acoustics can be written in the form

$$u_t + uu_x = \mathscr{H}(x, t; u, \ldots), \tag{2.7}$$

where $\mathscr{H}(x, t; u, \ldots)$ is a term linear in u representing some physical mechanism. For any initial disturbance containing forward-facing slopes, the effect of nonlinearity is to steepen these slopes, making apparently small linear effects significant in determining the overall waveform. In the absence of any linear mechanism (that is $\mathscr{H} \equiv 0$), multi-valued solutions appear in finite time (see §4) and the wave appears to overturn. Thus some previously ignored physical process must in fact become important to ensure

physically realistic solutions. From (2.3) and the known general solution of the initial-value problem for Burgers' equation, it is clear that the inclusion of thermoviscosity always ensures that single-valued wave solutions are obtained, but it is not immediately obvious whether or not the inclusion of relaxation or wall effects without molecular diffusivity in the fluid interior is sufficient to prevent wave overturning. Sugimoto (1990, 1991) concluded that the wall friction was not always sufficient, and that thermoviscosity becomes significant in resolving a Taylor-like viscous sub-shock. For the relaxing gas equation (2.6) it is clear that if $\Gamma = 0$ then (2.2) is obtained and overturning occurs, and that if $\Omega = 0$ (with $\Gamma \neq 0$) then Burgers' equation (2.3) is obtained, giving single-valued solutions at all finite times. Hence for a given initial wave profile, the parameter plane (Γ, Ω) must divide into regions for which the waveform remains single-valued and regions for which multi-valued solutions arise (in which case thermoviscosity then becomes vital in determining the actual waveform). In order to determine these regions of parameter space, a method is formulated in the next section which is able to distinguish between the occurrence of actual wave overturning in the model equation, and the appearance of small regions where the solution changes rapidly but remains single-valued. The remainder of this first paper is concerned with validating such an approach. Then in Part 2, the specific problem for relaxing gases, discussed above, is analysed in detail.

3. Intrinsic coordinate formulation

In the previous section, we introduced a number of model equations for the propagation of nonlinear waves including different attenuation and dispersion mechanisms and asked whether the inclusion of different effects can produce acceptable solutions. In this section we introduce a method for investigating the phenomenon of wave overturning by re-expressing the waveform in terms of intrinsic coordinates.

For a function $u(x)$, the angle $\psi(x)$ of the tangent to the graph of $u(x)$ can be obtained at any point, together with the arclength $s(x)$ along the curve from some fixed point x_0, by

$$\psi(x) = \tan^{-1}(u_x), \qquad s(x) = \int_{x_0}^{x} (1+u_x^2)^{\frac{1}{2}}\,\mathrm{d}x. \tag{3.1}$$

An alternative description of the original curve is then obtained by eliminating x between equations (3.1) to give the tangent angle in terms of arclength, $\psi = \psi(s)$. If in addition the value of the original function is specified at the fixed point this new 'intrinsic' description uniquely defines the original curve, by means of the equations

$$u(s) = u(x_0) + \int_0^s \sin\psi(s)\,\mathrm{d}s, \qquad x(s) = x_0 + \int_0^s \cos\psi(s)\,\mathrm{d}s. \tag{3.2}$$

For any continuous, non-branching curve, $\psi(s)$ will be single-valued throughout. It is for this reason that intrinsic coordinates prove useful in investigating wave overturning; the appearance of a multi-valued wave solution (catastrophe) corresponds simply to the absolute value of the 'intrinsic function' $\psi(s,t)$ exceeding $\frac{1}{2}\pi$ for some s.

The nonlinear wave equations of interest (§2) can all be written in the form

$$u_t + uu_x = \mathscr{H}(x, t; u, u_x, \ldots), \tag{3.3}$$

where $\mathscr{H}$ describes some linear process. The particular form of $\mathscr{H}$ dictates whether overturning will in fact occur. To investigate this possibility, the governing equation is

recast in intrinsic form and to do so we begin by transforming into intrinsic coordinate form the equation

$$u_t = F(x, t; u, u_x, \ldots), \tag{3.4}$$

the only restriction placed on F being that there should be no dependence on the time-derivatives of u. Choosing the fixed point on the curve as $x_0 = 0$, and writing $u(0, t)$ as $U(t)$, equation (3.2) becomes

$$u(s, t) = U(t) + \int_0^s \sin\psi(s, t)\,\mathrm{d}s, \qquad x(s, t) = \int_0^s \cos\psi(s, t)\,\mathrm{d}s. \tag{3.5}$$

Since $u_x = \tan\psi$, it follows that

$$\psi_t = \cos^2\psi u_{xt} = \cos^2\psi F_x. \tag{3.6}$$

Re-expressing this in terms of arclength gives

$$\psi_\tau + s_t\psi_s = \cos\psi f_s, \tag{3.7}$$

where $\partial/\partial\tau$ denotes differentiation with respect to time with s held constant, and $f(s, \tau) \equiv F(x, t; u, u_x, \ldots)$. Then from the definition of arclength,

$$\begin{aligned} s_t &= \int_0^x u_x u_{xt}(1 + u_x^2)^{-\frac{1}{2}}\,\mathrm{d}x = \int_0^x u_{xt}\sin\psi\,\mathrm{d}x \\ &= \int_0^s f_s \sin\psi\,\mathrm{d}s. \end{aligned} \tag{3.8}$$

Thus the evolution of $\psi(s, \tau)$ is given by

$$\psi_\tau = f_s\cos\psi - \psi_s\int_0^s f_s\sin\psi\,\mathrm{d}s. \tag{3.9}$$

This, together with the relation $U_\tau = f(0, \tau)$, is the intrinsic form of (3.4).

Returning to the general nonlinear wave equation (3.3), the intrinsic form becomes

$$\psi_\tau = -\sin^2\psi - \psi_s\int_0^s \sin\psi\cos\psi\,\mathrm{d}s - \psi_s U\sec\psi_0 + h_s\cos\psi - \psi_s\int_0^s h_s\sin\psi\,\mathrm{d}s, \tag{3.10a}$$

which, by integration by parts, can be written in the alternative form

$$\begin{aligned} \psi_\tau = -\sin^2\psi - \psi_s\int_0^s \sin\psi\cos\psi\,\mathrm{d}s - \psi_s U\sec\psi_0 \\ + \psi_s h_0\sin\psi_0 + (h\cos\psi)_s + \psi_s\int_0^s (h\cos\psi)\,\psi_s\,\mathrm{d}s, \end{aligned} \tag{3.10b}$$

together with the equation governing $U(\tau)$,

$$U_\tau = -U\tan\psi_0 + h_0. \tag{3.11}$$

Here the suffix 0 refers to the value of the function at $s = 0$ and h represents the attenuation or dispersion function, but re-expressed in terms of s and τ (and dependent on $\psi(s, \tau), \psi_s(s, \tau)$ etc.) rather than x and t (and involving $u(x, t), u_x(x, t)$ etc.). In terms of the notation previously introduced, $h(s, \tau) \equiv \mathscr{H}(x, t; \ldots)$. Thus, given an initial waveform $u(x, 0)$, the intrinsic function $\psi(s, 0)$ and $U(0)$ can be obtained from (3.1) and (3.5), and then (3.10) and (3.11) give ψ and U at later times.

When considering the evolution of a step transition, the boundary condition is that $\psi \to 0$ as $|s| \to \infty$, but for a periodic disturbance the conditions are more complicated. Evidently, the intrinsic function $\psi(s,\tau)$ will be spatially periodic, but with a time-dependent period $S(\tau)$. Setting $f = h - u\tan\psi$ in (3.8), integration by parts gives

$$S_\tau = \int_0^S \sin\psi\cos\psi\,\mathrm{d}s + \int_0^S h_s \sin\psi\,\mathrm{d}s. \tag{3.12}$$

Thus the evolution of a periodic disturbance is governed, in intrinsic form, by the set of three differential equations (3.10)–(3.12). The complicated form of these equations suggests that analytical progress is likely to be limited. The problems to be faced can be seen simply by considering the initial condition. Putting $u_0(x) = \sin x$ we find that $\psi(s,0)$ is given implicitly by

$$s = \sqrt{2}\,\mathrm{E}(\cos^{-1}[\tan\psi], 1/\sqrt{2}), \tag{3.13}$$

where $\mathrm{E}(y,k)$ is the elliptic integral of the second kind (see, for example, Abramowitz & Stegun 1965). The other initial conditions then become

$$S(\tau = 0) = \sqrt{2}\,\mathrm{E}(2\pi, 1/\sqrt{2}), \quad U(\tau = 0) = 0. \tag{3.14}$$

Progress does not seem much more likely even in the case of step transitions or isolated pulses, when essentially only one differential equation must be solved. For this reason, the remainder of this paper is concerned with the *numerical* solution of these equations and with the relation between the numerical solutions and the asymptotic and exact properties of the equations in the original (x,t) variables.

4. Numerical implementation and results

The two classes of disturbances described in the previous section are now considered separately.

4.1. *Periodic disturbances*

For convenience, the three equations to be solved are rewritten here along with the boundary conditions;

$$\left.\begin{aligned}
&\psi_\tau = -\sin^2\psi - \psi_s \int_0^s \sin\psi\cos\psi\,\mathrm{d}s - \psi_s U\sec\psi_0 + h_s\cos\psi - \psi_s\int_0^s h_s\sin\psi\,\mathrm{d}s,\\
&U_\tau = -U\tan\psi_0 + h_0,\\
&S_\tau = \int_0^S \sin\psi\cos\psi\,\mathrm{d}s + \int_0^S h_s\sin\psi\,\mathrm{d}s,\\
&\psi(0,\tau) = \psi(S(\tau),\tau), \qquad \psi_s(0,\tau) = \psi_s(S(\tau),\tau), \text{ etc.}
\end{aligned}\right\} \tag{4.1}$$

The periodicity of ψ with respect to s at fixed time naturally suggests spectral evaluation of spatial derivatives. This method of evaluating derivatives is well known, though the essential points are repeated here. The most important thing to note is that the spatial grid must consist of equally spaced mesh points.

Consider first a function $V(x,t)$ with period X in x. In order to evaluate V_x by spectral methods, V must be known at N equally spaced mesh points given by

$$x_j = jX/N, \quad j = 0, 1, \ldots, N-1. \tag{4.2}$$

The finite Fourier transform is then defined by

$$\hat{V}(k,t) = \frac{1}{N}\sum_{j=0}^{N-1} V(x_j,t)\,\mathrm{e}^{-\mathrm{i}2\pi k x_j/N}, \tag{4.3}$$

where $$k = -\tfrac{1}{2}N+1,\ldots,\tfrac{1}{2}N,$$

with inverse transform

$$V(x_j,t) = \sum_{k=-\frac{1}{2}N+1}^{\frac{1}{2}N} \hat{V}(k,t)\,\mathrm{e}^{\mathrm{i}2\pi k x_j/N}. \tag{4.4}$$

The spatial derivatives immediately follow as

$$V_x(x_j,t) = \sum_{k=-\frac{1}{2}N+1}^{\frac{1}{2}N} \frac{\mathrm{i}2\pi k}{N}\hat{V}(k,t)\,\mathrm{e}^{\mathrm{i}2\pi k x_j/N}, \tag{4.5}$$

and so on.

As well as ensuring the periodicity of all the derivatives, the method of calculation gives accurate values for each derivative. Of course, if rapid variation of V with x arises in the evolution, more spectral components must be used to ensure that this accuracy is maintained. The integrals of the periodic functions are evaluated in terms of spectral components by taking the transform of the whole integrand. Computation of these quantities can be carried out efficiently by the use of a fast Fourier transform (FFT) algorithm, with the number of mesh points set to 2^n (with n an integer) for optimal speed.

Returning to the current problem, suppose that at time t_j, $S(\tau_j)$ and $U(\tau_j)$ are known, together with $\psi(s_{i,j},\tau_j)$, at *equally spaced* mesh points

$$s_{i,j} = (i/N)\,S(\tau_j), \quad i = 0,1,\ldots,N, \tag{4.6}$$

with $\psi(s_{N,j},\tau_j) = \psi(s_{0,j},\tau_j)$. Then the first-order time derivatives are obtained from (4.1), and ψ, S and U are advanced in time by forward difference,

$$\psi(s_{i,j},\tau_{j+1}) = \psi(s_{i,j},\tau_j) + \Delta\tau\psi_\tau(s_{i,j},\tau_j). \tag{4.7}$$

However $s_{i,j} \neq s_{i,j+1}$ unless $S_\tau(\tau_j) = 0$, and therefore in general $\psi(s_{i,j+1},\tau_{j+1})$ must be obtained by interpolation from $\psi(s_{i,j},\tau_{j+1})$. This is accomplished using a standard interpolation package based on Aitken's technique of successive linear interpolation. Alternatively, the need for this interpolation can be eliminated by rescaling the spatial range to the interval [0, 1] with the evolution equations recast in terms of $z = s/S$. This simplification is at the expense of making the set of governing equations more complicated, but a reduction in computation time of about 5% is obtained.

When implementing this simple numerical scheme, care must be taken in defining the spatial resolution and in choosing a suitable time step. A full stability analysis of the intricate set of governing equations appears to be impractical. Instead, an *ad hoc* testing procedure was introduced into the numerical evaluation. A spectral component was considered if its magnitude, relative to the principal component, was greater than 5×10^{-4}. Writing the ith spectral components as $\hat{\psi}^{(i)}$, the evolution of these components should be accurately predicted if their relative changes in magnitude at each time step are small. To comply with this, we adjust the size of the time step $\Delta\tau$ to satisfy the condition

$$\max_i\left(\frac{\hat{\psi}_\tau^{(i)}\,\Delta\tau}{\hat{\psi}^{(i)}}\right) < 0.2, \tag{4.8}$$

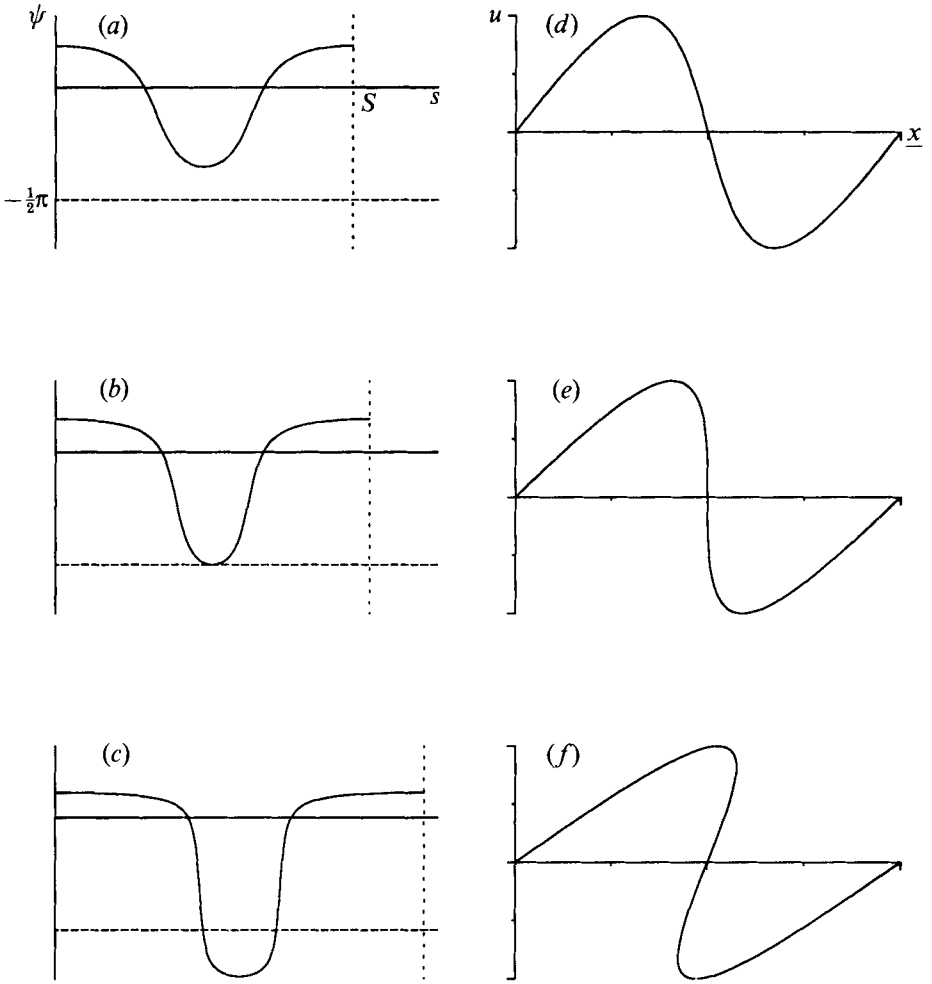

FIGURE 1. The evolution of a periodic solution to the inviscid Burgers equation (2.2) using intrinsic coordinates (*a–c*), together with the corresponding physical waveforms (*d–f*). Exact results for the physical waveform obtained by the method of characteristics are also plotted in (*d–f*), but are indistinguishable from the solutions obtained using intrinsic coordinates. (*a*, *d*) $t = 0.5$; (*b*, *e*) $t = 1.0$; (*c*, *f*) $t = 1.75$.

with the maximum being taken over the set of all significant components. The spatial resolution must be chosen such that all the significant spectral components are accurately determined. For an initially sinusoidal wave profile, it is found that the resulting intrinsic description is a smooth function and so, at first, 64 Fourier modes are sufficient to include all the significant components. In Part 2, where this method will be applied to equations of physical interest, it is seen that as the wave evolves, the intrinsic solution develops structure of a much finer scale. To allow for this, the number of mesh points should be doubled as soon as the significant component with the highest wavenumber approaches the maximum wavenumber included at that stage. In the most extreme cases dealt with in Part 2, 1024 spectral components were considered.

By adjusting the spatial and temporal step sizes in the fashion outlined above, it is hoped that accurate solutions to the model equations of §2 will be obtained. In the rest of this section we investigate this accuracy. One simple check on the accuracy of the

scheme is obtained by considering the value of $\int_0^s \cos\psi \, ds$. This is not explicitly conserved in the numerical scheme, but should always be equal to the wave period, 2π. In all the cases computed, the error was less than 0.1 %. Apart from this, accuracy can be tested by looking at equations of the form (1.1) for which exact solutions are available. The validity of the method in dealing with waves which do in fact overturn can be demonstrated by considering $\mathscr{H} = 0$, corresponding to nonlinear evolution with no attenuation or dispersion. In this case exact solutions can be obtained by the method of characteristics, namely

$$u(x, t) = u_0(z)$$

with $z(x, t)$ given implicitly by

$$z = x + tu_0(z),$$

which, in the case of an initial sinusoidal wave $u_0(z) = \sin z$, gives multi-valued solutions for $t > 1$. In figure 1 the intrinsic wave function $\psi(s, t)$ is plotted before wave overturning (figure 1*a*), at the point of overturning (figure 1*b*), and well after overturning (figure 1*c*), together with the corresponding physical waveforms $u(x, t)$ (figure 1*d–f*) deduced from the intrinsic representation. The exact solutions to the physical equation, obtained by the method of characteristics, are also plotted on the latter set of plots but are indistinguishable from the numerical solution. At time $t = 1.5$, corresponding to figure 1(*c*, *f*) when the wave is fully overturned, the intrinsic solution obtained numerically is converted back to physical space, and then compared with the exact solution by characteristics. The relative accuracy, expressed as the absolute error relative to the wave amplitude, is found to be better than 0.2% everywhere. At earlier times, prior to wave overturning, a very similar degree of accuracy was obtained.

Before claiming that this numerical scheme is completely valid, one should note from figure 1 that the intrinsic solution remains a fairly smooth function of s. To test the more demanding case when $\psi(s)$ becomes less smooth, a small amount of thermoviscous dissipation was included. The solution should then remain single-valued throughout, with a narrow shock region inserted. The inner detail of the shock region should be described well by intrinsic coordinates, but at both extremes of this region there is rapid change in the slope of the wave. For a (scaled) diffusivity $\Delta = 0.05$ (as in (2.3)), the solutions obtained via intrinsic coordinates are plotted in figure 2. These solutions are plotted at the same times as in figure 1, allowing direct comparison of the inviscid and the viscous wave evolution. Figure 2(*a–c*) shows the intrinsic wave function and figure 2(*d–f*) shows the corresponding physical waveforms. Comparing figures 1 and 2, it can be seen that with a small coefficient of diffusivity, the waveform is virtually unaffected by viscosity until significant wave steepening has occurred. The viscous solution obtained numerically in this way can then be compared with the exact solution of (2.3) obtained by the Hopf–Cole linearizing transformation. At all times up to $t = 1.75$, the relative errors are found to be less than 0.3 %. As in figure 1, the exact solutions are also plotted at each time in figure 2(*d–f*), and in each case the two curves are indistinguishable.

The main motivation behind the intrinsic coordinate formulation was to investigate the conditions under which wave overturning does occur. The accuracy in prediction of the time of overturning can be tested by looking at the solution of the Varley–Rogers equation (2.4). Solving by the method of characteristics, it can be shown that for a unit-amplitude sinusoidal wave, overturning occurs if $\alpha < 1$, at time

$$t_\alpha = -\ln(1-\alpha)/\alpha. \tag{4.9}$$

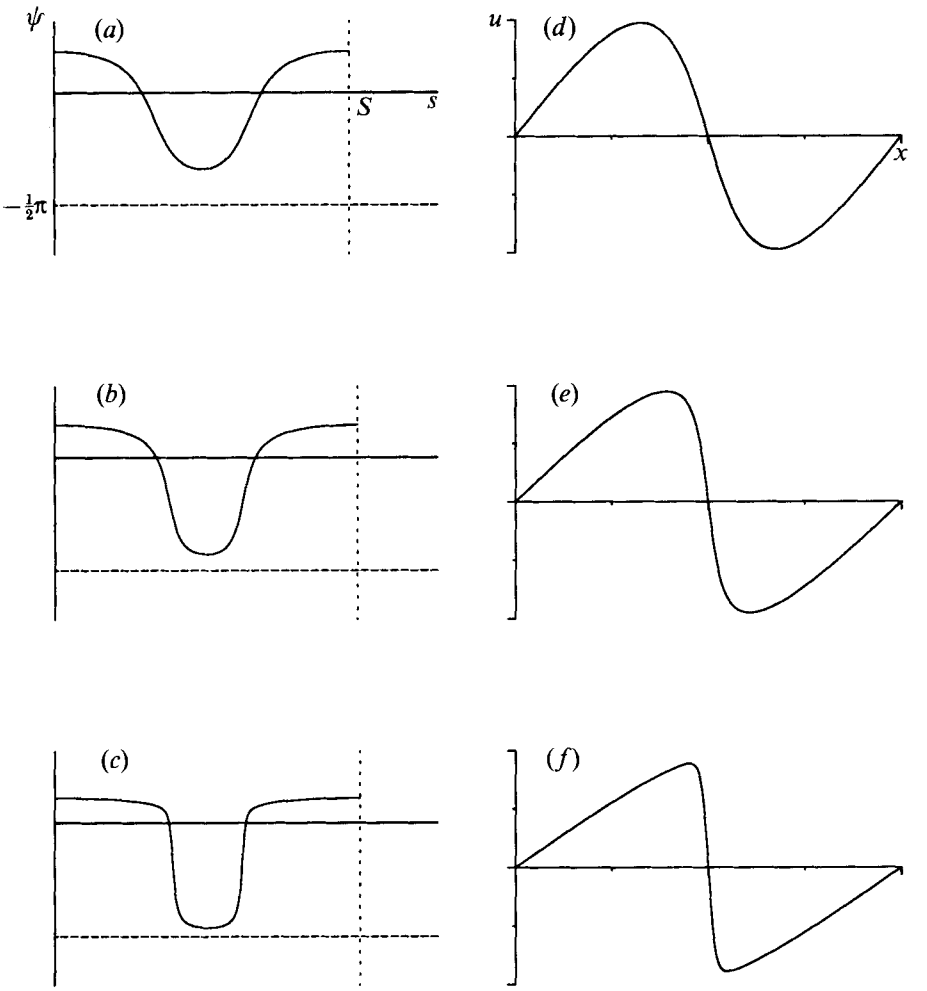

FIGURE 2. The evolution of a periodic solution to the Burgers equation (2.3), with $\Delta = 0.05$, using intrinsic coordinates (*a–c*), together with the corresponding physical waveforms (*d–f*). Exact results for the physical waveform obtained using the Hopf–Cole transformation are also plotted in (*d–f*), but are indistinguishable from the solutions obtained using intrinsic coordinates. (*a, d*) $t = 0.5$; (*b, e*) $t = 1.0$; (*c, f*) $t = 1.75$.

Comparing the numerical values of t_α, obtained using intrinsic coordinates, with (4.9) for various values of $\alpha < 1$ reveals agreement to at least four significant figures.

In each of the cases considered so far, the linear mechanism represented by $\mathscr{H}$ is reasonably simple even when converted to its intrinsic coordinate form. Also, the equations have been non-dispersive and hence $U_t = 0$ throughout. In Part 2, accuracy checks will be described for propagation through a relaxing medium. Numerical results obtained from the intrinsic coordinate formulation will be compared with solutions obtained directly from the physical equation (2.6) using a pseudo-spectral scheme.

4.2. *Step transitions*

When considering the evolution of either step transitions or isolated pulses, only one differential equation need be solved, since by suitable choice of the fixed point for the intrinsic coordinates, U will be constant. The boundaries of the computational domain

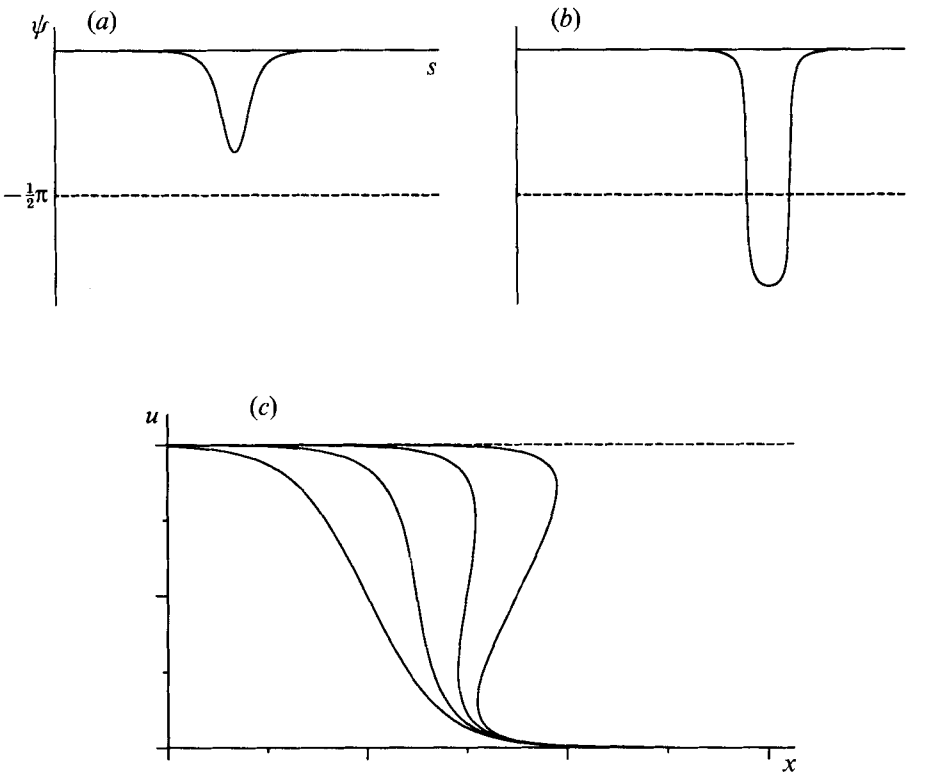

FIGURE 3. The propagation of a step-like transition governed by the inviscid Burgers equation (2.2) as calculated using intrinsic coordinates (*a*, *b*), together with the resulting evolution of the physical waveform (*c*). Exact results obtained using the method of characteristics are also plotted in (*c*), but are indistinguishable from the results obtained using intrinsic coordinates. (*a*) $t = 1.0$, (*b*) $t = 3.0$, (*c*) $t = 0, 1.0, 2.0, 3.0$.

are taken well away from the region of interest, so that the boundary conditions become $\psi = 0$, $\psi_s = 0$, etc. A straightforward explicit finite-difference scheme was then used, although the pseudo-spectral method outlined at the beginning of this section may also be used. Since steadily translating solutions for step transitions are generally well known, only a few cases were computed in order to demonstrate the applicability of the intrinsic coordinate method. The accuracy of the numerical scheme was tested by changing both spatial and temporal step sizes and by comparison with the exact solutions for inviscid and viscous propagation. For the numerical investigation, the initial profile describing a transition between $u = 1$ as $x \to -\infty$ and $u = 0$ as $x \to \infty$ was taken to be

$$u_0(x) = \frac{1}{2}\left[1 - \tanh\left(\frac{x - x_*}{\lambda}\right)\right], \tag{4.10}$$

with $x_* = 4.0$, the 'centre' of the profile, and $\lambda = 0.75$, the width of the transition. At $x = 0$, $u_0 \approx 1 - 1 \times 10^{-5}$, and so $x = 0$ is taken as the fixed point for the intrinsic coordinate formulation, with $U(t)$ kept fixed and equal to unity.

The inviscid results are given in figure 3. Figure 3(*a*, *b*) shows the intrinsic wave function at $t = 1$ and 3 respectively, while figure 3(*c*) shows the evolution of the physical wave profile from $t = 0$ to 3. Comparing these numerical results with the characteristic solution at $t = 3$, which is after the wave has overturned, the relative

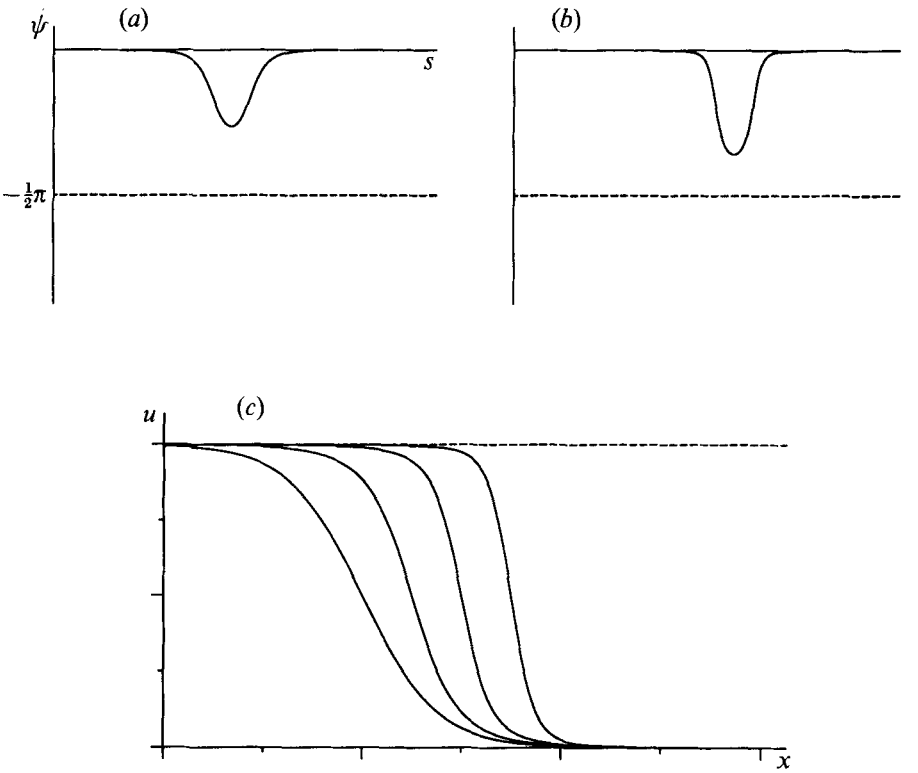

FIGURE 4. The propagation of a step-like transition governed by the Burgers equation (2.3), with $\Delta = 0.05$, as calculated using intrinsic coordinates (*a*, *b*), together with the resulting evolution of the physical waveform (*c*). Exact results obtained using the Hopf–Cole transformation are also plotted in (*c*), but are indistinguishable from the results obtained using intrinsic coordinates.

error is found to be less than 0.2%, and when plotted together in figure 3(*c*), the two solutions are indistinguishable. In figure 4 results for viscous propagation, governed by Burgers' equation, are plotted at the same times as figure 3. The results can be compared with the exact Hopf–Cole solution, revealing relative errors of less than 0.25%. If figures 3 and 4 are compared, the effect of viscosity on the intrinsic wave function can be seen. At small t, $|\psi|$ is still well away from $\frac{1}{2}\pi$ and, since the coefficient of diffusivity is small ($\Delta = 0.05$), the effect of viscosity is negligible. At $t = 1.0$, the effect of viscosity is still small and the intrinsic functions are very similar, except right in the middle of the shock (figures 3*a*, 4*a*). At later times when much steeper spatial gradients appear, viscosity becomes significant and its presence prevents $|\psi|$ exceeding $\frac{1}{2}\pi$ (i.e. no wave overturning occurs).

Taken together, these accuracy checks validate the general method and allow sample calculations to be undertaken for relaxing gases. In cases where overturning occurs, computation becomes very difficult once the wave profile is well past the point of overturning, and for more detailed analysis of such situations, a more sophisticated numerical scheme would no doubt be desirable. For the physical problems we have in mind, however, there is less interest in that aspect than in the question of whether overturning does in fact occur in finite time or not, and to answer that question the present scheme seems reliable.

5. Conclusion

In this paper we have introduced a new method for investigating the appearance of multi-valued solutions in nonlinear wave propagation. Although such solutions are physically meaningless in an acoustics context, it is important to be able to identify their occurrence as an indication of the inadequacy of the model governing equation. Conventional solution methods generally fail as the wave approaches the point of overturning, so a new method of describing the wave profile is introduced. The essential point is that spectral and difference methods are fundamentally incapable of producing triple-valued solutions in the configuration space. Accordingly some alternative representation of the waveform is necessary, which effectively unfolds the triple-valued wave. By reformulating the whole problem in terms of *intrinsic coordinates*, the objective is achieved, and the wave shape well past the point of overturning can be obtained. The validity of such a method is amply demonstrated by comparison of numerical solutions obtained in this way with exact solutions. As well as being able to cope with wave overturning, numerical implementation of the intrinsic coordinate formulation automatically resolves narrow regions of rapid change in the wave amplitude, by concentrating mesh points in such regions. However, this does not necessarily allow a reduction in the number of mesh points required, since regions of rapid change in wave slope must be resolved. One disadvantage of the intrinsic coordinate method is that one reasonably simple nonlinear wave equation is converted to a much more complicated set of equations, but from a numerical point of view that is irrelevant.

Previous work on wave overturning has been largely in connection with surface water waves, when wave breaking is physically meaningful. Longuet-Higgins & Cokelet (1976) map the free surface to a complex plane then use intrinsic coordinates; however, these do not correspond to the arclength and slope of the physical waveform. In a series of papers Meyer (1986*a–c*) considered the phenomenon of water wave breaking on gentle beaches. In the system of equations studied, explicit Riemann invariants were obtained, and by using these as independent variables, the well-known Euler–Poisson–Darboux (or EPD) equation was obtained. Meyer was able to prove several existence and inversion theorems relating solutions of the EPD equation (labelled 'apparent solutions'), to the existence, or otherwise, of single-valued solutions of the original beach equations. In the class of problems addressed in the current paper, no explicit Riemann invariants are in general available and hence it is not clear how the analysis of Meyer can be readily modified for these cases.

Part 2 presents an analysis of the interplay between thermoviscous diffusion, relaxation and nonlinearity using the methods described here. For certain relaxation parameter values, it is found that some other physical process (such as thermoviscous diffusion) must become significant, though only in a very restricted portion of the wave form. Using other methods of solution, this subtlety in the wave profile may well be overlooked.

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