Reaction-diffusion equations.

For a chemical in a long tube, in which the problem can be reduced to one spatial dimension x, the reaction-diffusion equation for the density u is

$$(*) \qquad u_t = \gamma u_{xx} + R(u)$$

Let us take $\gamma = 1$ and $R(u) = u(1-u^2)$ [the Newell-Whitehead-Segel equation] and seek traveling solutions

$$u(x,t) = v(x-mt).$$

With this ansatz, equation $(*)$ gives

$$v'' + mv' + v(1-v^2) = 0,$$

and, with $w = v'$, this is equivalent to the system

$$(**) \qquad \begin{aligned} v' &= w, \\ w' &= -mw - v(1-v^2). \end{aligned}$$

The constant solutions of this equation are $w(\xi) = 0$ and

$$v(\xi) = v_0 = -1, 0, 1,$$

which give $u(x,t) = v_0$. The solutions $v_0 = \pm 1$ are not stable, as analysis of the system $(**)$ shows.

The linearization of this system about $(v,w) = (0,0)$ is

$$\begin{bmatrix} v' \\ w' \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ -1 & -m \end{bmatrix} \begin{bmatrix} v \\ w \end{bmatrix} + \mathcal{O}(v^2+w^2),$$

and the eigenvalues of this matrix are

$$\lambda = \frac{1}{2}\left[-m \pm \sqrt{m^2-4}\right].$$

The linearization about $(v,w) = (\pm 1, 0)$ is

$$\begin{bmatrix} v' \\ w' \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 2 & -m \end{bmatrix} \begin{bmatrix} v \mp 1 \\ w \end{bmatrix} + \mathcal{O}\left((v \mp 1)^2 + w^2\right),$$

with associated eigenvalues

$$\lambda = \frac{1}{2}\left[-m \pm \sqrt{m^2+8}\right].$$

Thus, the fixed points $(\pm 1, 0)$ are unstable, with a 1D stable manifold.

<u>Case $m=0$</u> : There are periodic solutions, which traverse level sets of $\mathcal{E}(v,w) = \frac{1}{2}w^2 + \frac{1}{2}v^2 - \frac{1}{4}v^4$:

$$\frac{d\mathcal{E}}{d\xi} = \frac{\partial \mathcal{E}}{\partial v} v' + \frac{\partial \mathcal{E}}{\partial w} w' = (v - v^3)v' + ww' = (v-v^3)w + w(-v(1-v^2)) = 0$$

These give <u>equilibrium</u> solutions $u(x,t) = v(x)$ of $(*)$, so the <u>reaction balances the diffusion</u> exactly.

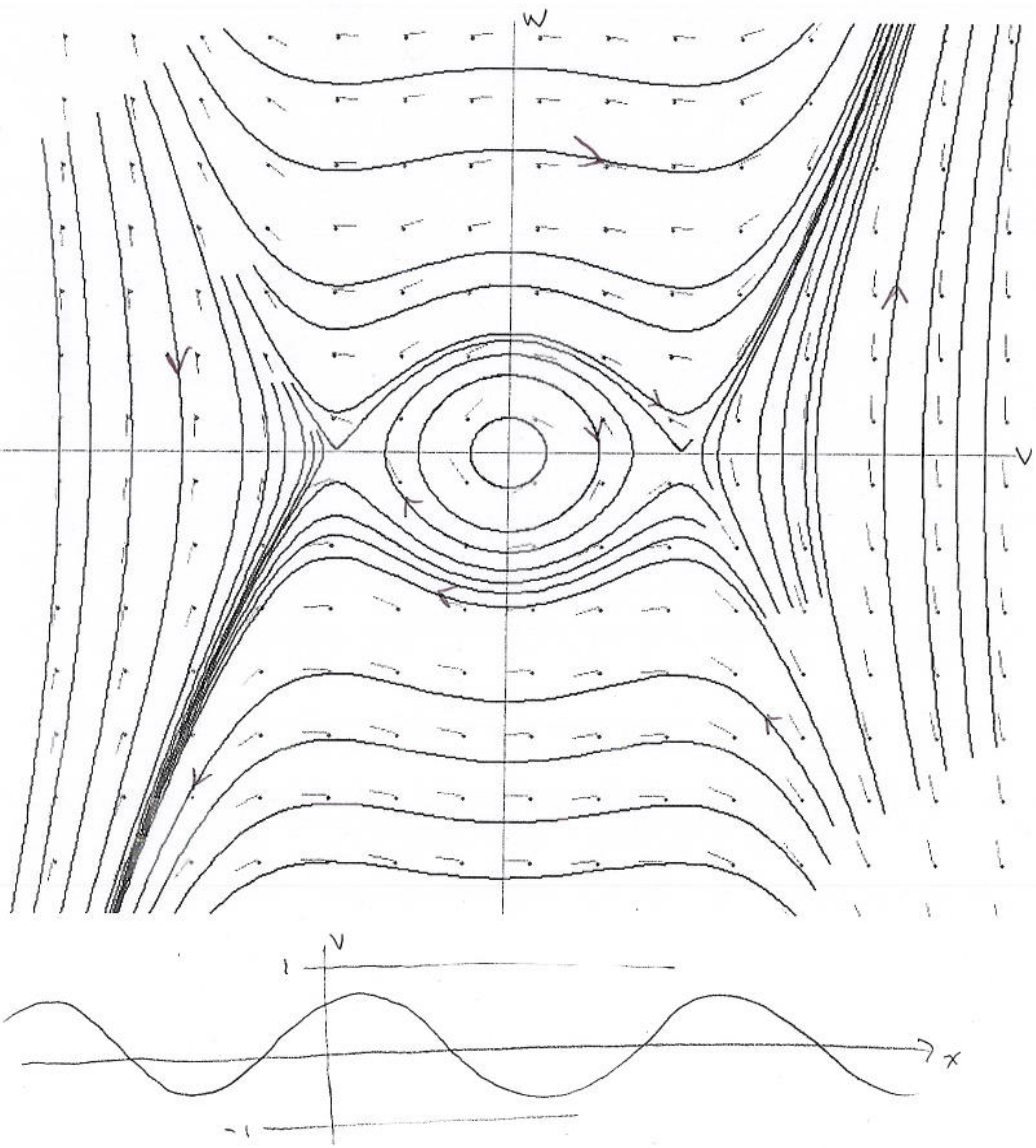
<u>Case $m>0$</u> : There are solutions $v(\xi)$ that decay as $\xi \to \infty$, that is, in the direction of propagation, $u(x,t) = v(x-mt) \to 0$ as $x \to \infty$

They also oscillate if $m<2$

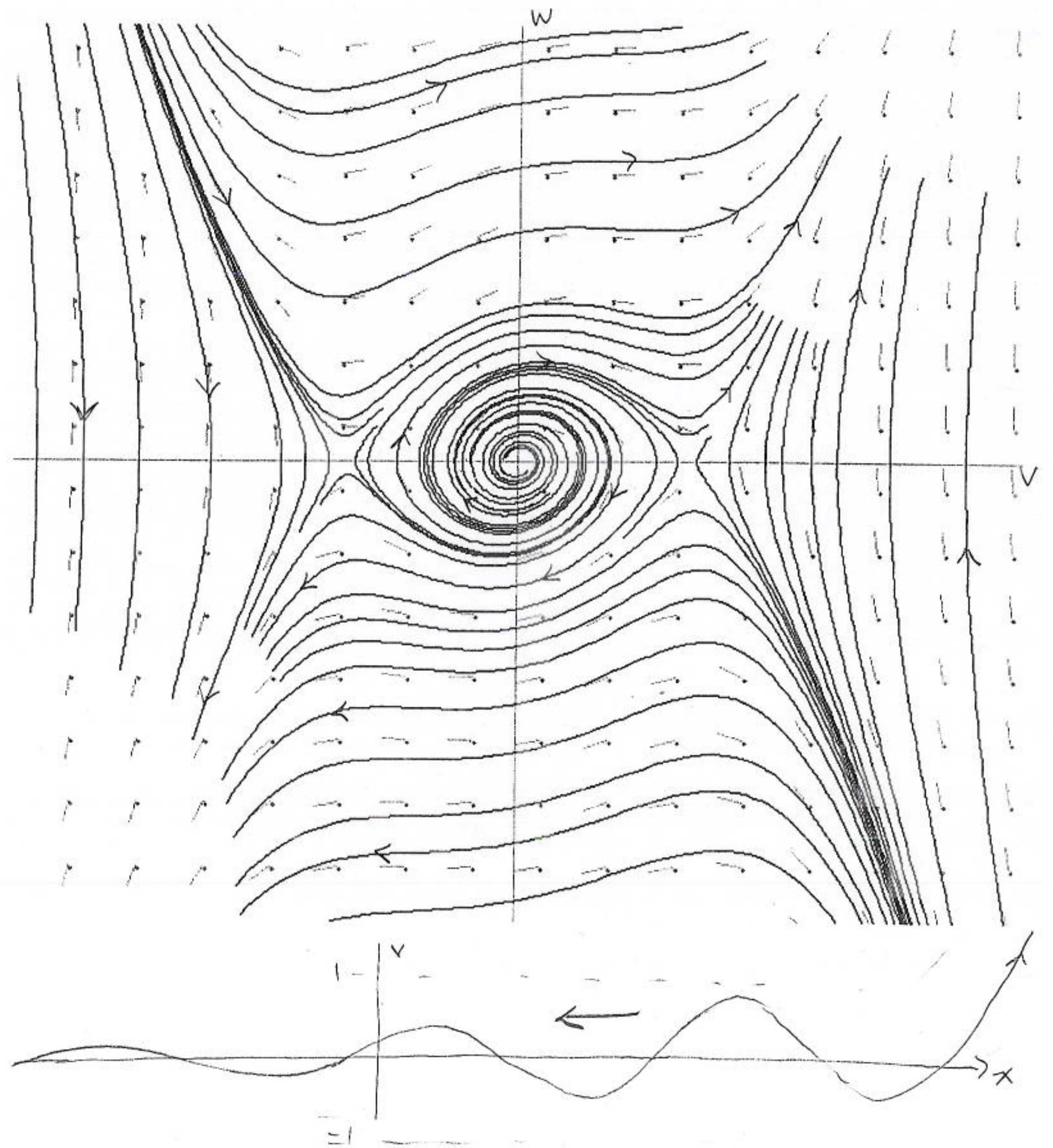
<u>Case $m<0$</u> : $\exists$ solutions that decay as $x \to -\infty$, again in the direction of propagation.

[These phase portraits were done with the applet at www.math.psu.edu/melvin/phase/newphase.html]

$m = 0$. The closed orbits give periodic equilibrium solutions $u(x,t) = v(x)$, for which diffusion exactly balances reaction

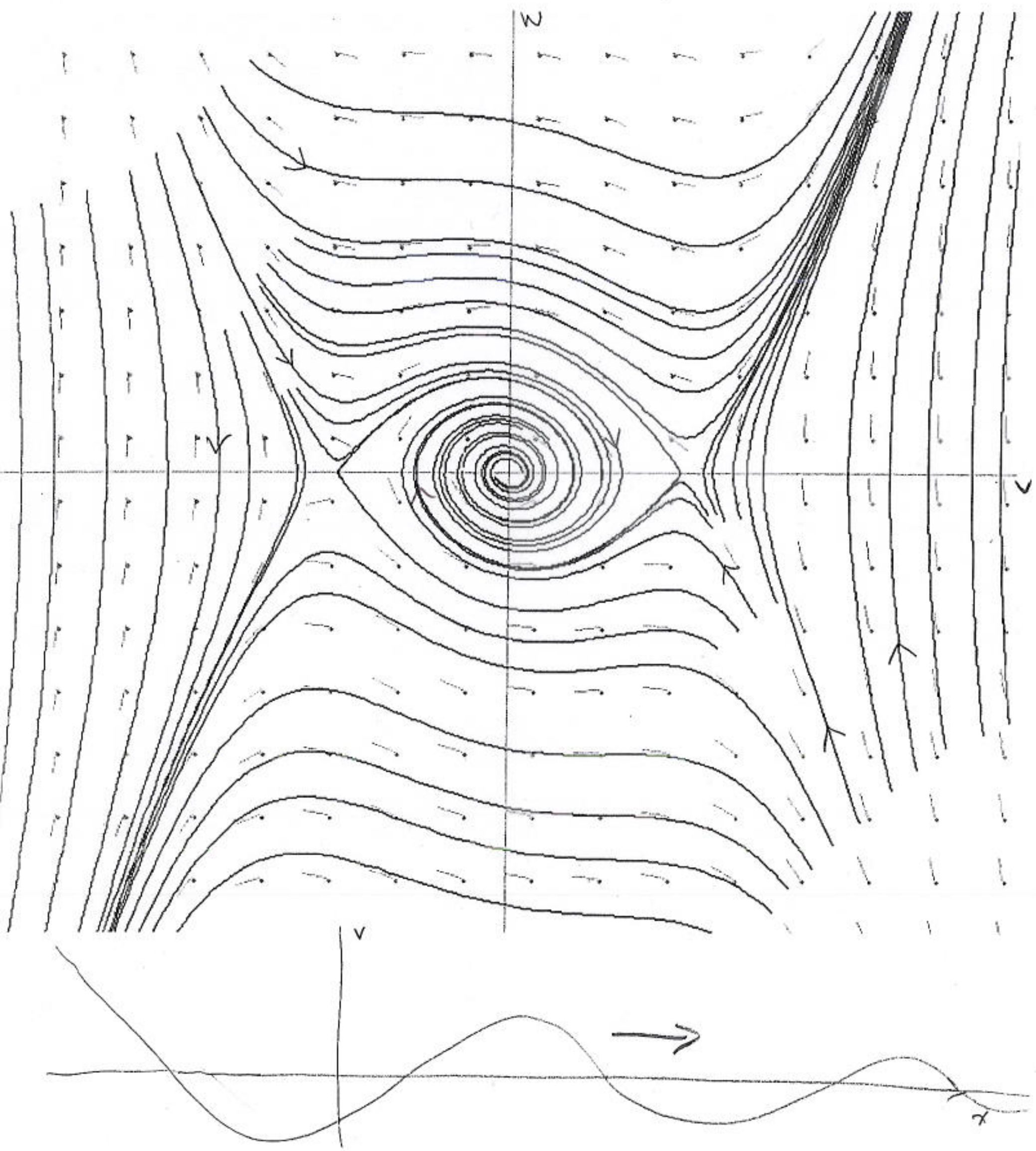


$m = -0.2$: Backward-traveling solutions decay as $x \to -\infty$, that is, in the direction of travel; they also oscillate for x suff. large

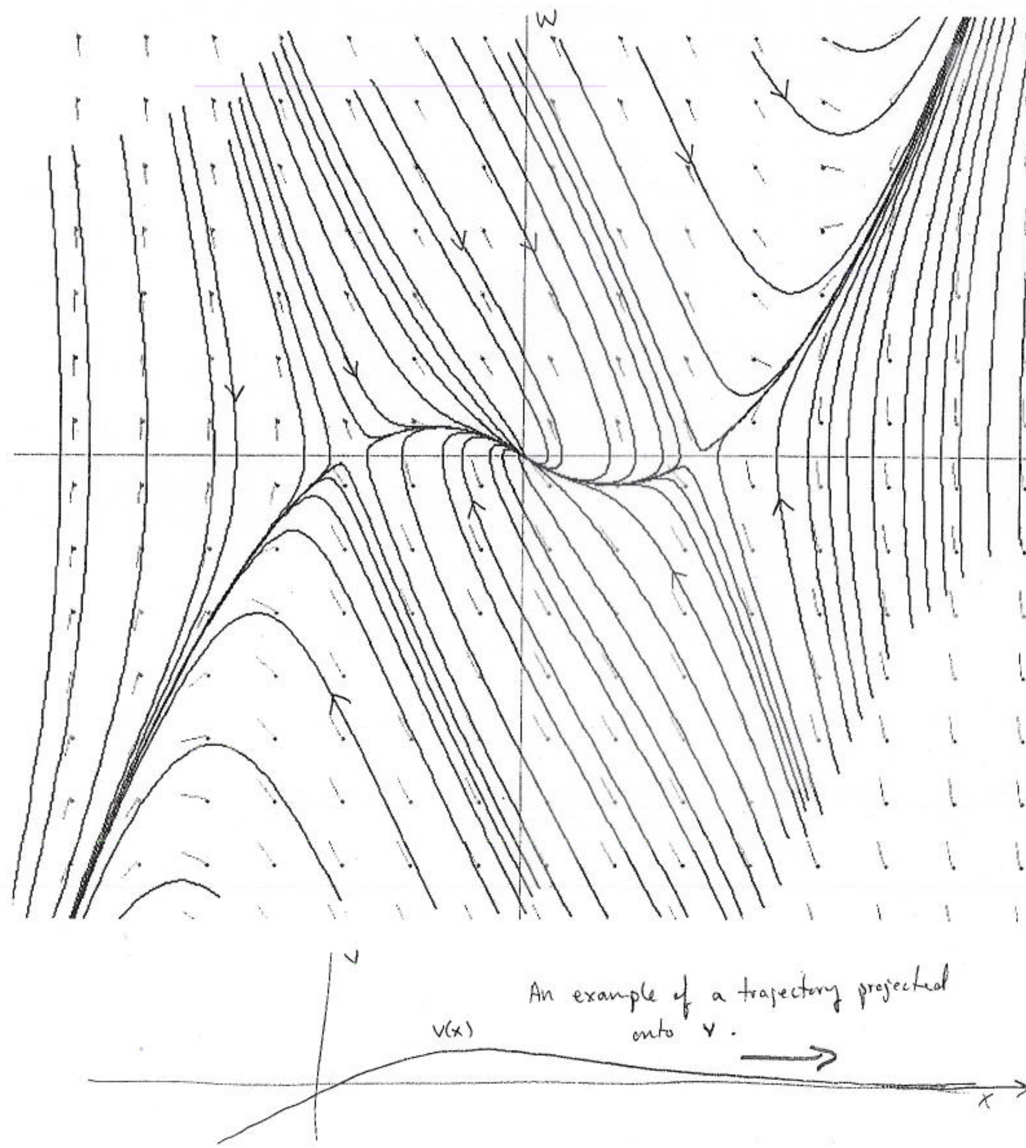


Some forward-traveling solutions $u(x,t) = v(x - 0.2t)$ decay

$m = 0.2$: as $x \to \infty$, and oscillate.



$m = 2.1$: No oscillations.



An example of a trajectory projected onto V.

Nonlinear advection

Let us return to the conservation law

$$\frac{\partial u}{\partial t} + \nabla_x \cdot F = 0$$

and consider a constitutive relation of the form

$$F = F(u),$$

that is, F is determined by the value of the density at each (x,t).

In the 1D case, this gives

$$(\dagger) \qquad u_t + F(u)_x = u_t + F'(u)\, u_x = 0.$$

The transport speed depends on u, so the equation is nonlinear (unless $F'(u)$ is constant). Set $F'(u) = c(u)$

The characteristic curves, which are solutions of

$$\frac{dx}{ds} = c(u), \quad x(0) = \xi$$
$$\frac{dt}{ds} = 1, \quad t(0) = 0$$

are not determined independently of the solution $u(x,t)$.

But what we know is that, by $(\dagger)$,

$$\frac{du}{ds} = 0,$$

so u is constant along these curves and so therefore $c(u)$ is also constant. This means that the characteristic curves in (x,t)-space are lines $\{x = \xi + c_\xi s, \ t = s\}$

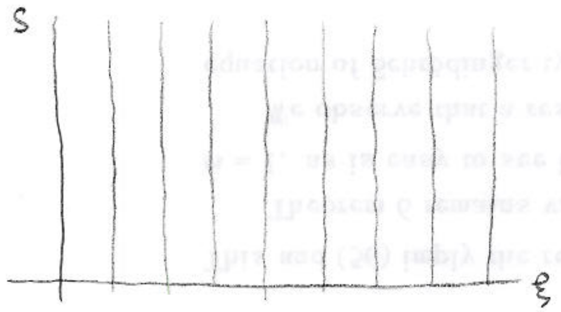
in which $c_\xi = u(x(0), t(0)) = u(\xi, 0)$, which we can set equal to an initial density $g(\xi)$:

$$u(x,0) = g(x).$$

Thus the characteristic curves are

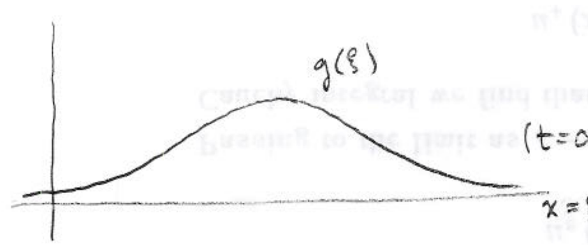
$$(\dagger\dagger) \quad \begin{cases} x = \xi + c(g(\xi))s, \\ t = s, \end{cases}$$

and u must be constant on each. This pair defines a transformation from (ξ, s) space to (x,t) space.



If a solution exists, it must have the form

$$u(x,t) = g(\xi). \quad (\dagger\dagger\dagger)$$

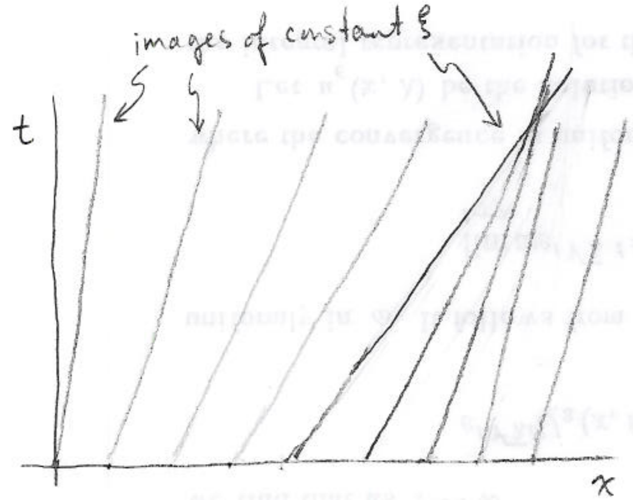


This makes sense if ξ is in fact a function of (x,t). We can determine the minimal value of s for which the map $(\xi, s) \mapsto (x,t)$ $(\dagger\dagger)$ is injective. Set $G(\xi) = c(g(\xi))$, and suppose

$$x_1 = \xi_1 + G(\xi_1)s,$$
$$x_2 = \xi_2 + G(\xi_2)s.$$

Then

$$x_1 = x_2 \iff s(G(\xi_2) - G(\xi_1)) + \xi_2 - \xi_1 = 0$$



The map $(\xi, s) \mapsto (\xi + c(f(\xi))s, s)$ for $c(u) = u$ and the given g.

This means, assuming $\xi_1 \neq \xi_2$,

$$s = -\frac{\xi_2 - \xi_1}{G(\xi_2) - G(\xi_1)} \quad \text{(which could be infinite)},$$

and the infemum of all such <u>positive</u> values of s, which we call s_*, is

$$s_* = \inf_{\xi_1 \neq \xi_2} \left\{ s = -\frac{\xi_2 - \xi_1}{G(\xi_2) - G(\xi_1)}, \ 0 < s \right\}$$

$$= \sup_{\xi_1 \neq \xi_2} \left\{ r = -\frac{G(\xi_2) - G(\xi_1)}{\xi_2 - \xi_1}, \ 0 \le r < \infty \right\}^{-1}.$$

If G is differentiable, then this is

$$s_* = \sup_{\xi \in \mathbb{R}} \left\{ r = -G'(\xi), \ 0 \le r < \infty \right\}^{-1} = \inf_{\xi \in \mathbb{R}} \left\{ s = -G'(\xi)^{-1}, \ 0 < s \right\}.$$

So the first time at which the transformation ceases to be injective is the reciprocal of the largest negative slope of $G(\xi)$.

Now, lets check that (††) really is a solution to (†) as long as the transformation (††) is differentiably invertible. Differentiating (††) with respect to t and x gives

$$0 = \xi_t (1 + G'(\xi)s) + G(\xi),$$
$$1 = \xi_x (1 + G'(\xi)s),$$

and, with $s = t$, we obtain

$$(1 + G'(\xi)t)(\xi_t + G(\xi)\xi_x) = 0,$$

and, for $t < s_*$, $1 + G'(\xi)t \neq 0$ so that

$$\xi_t + G(\xi)\xi_x = 0$$

The form $u(x,t) = g(\xi)$ implies

$$u_t = g'(\xi)\xi_t ,$$
$$u_x = g'(\xi)\xi_x ,$$

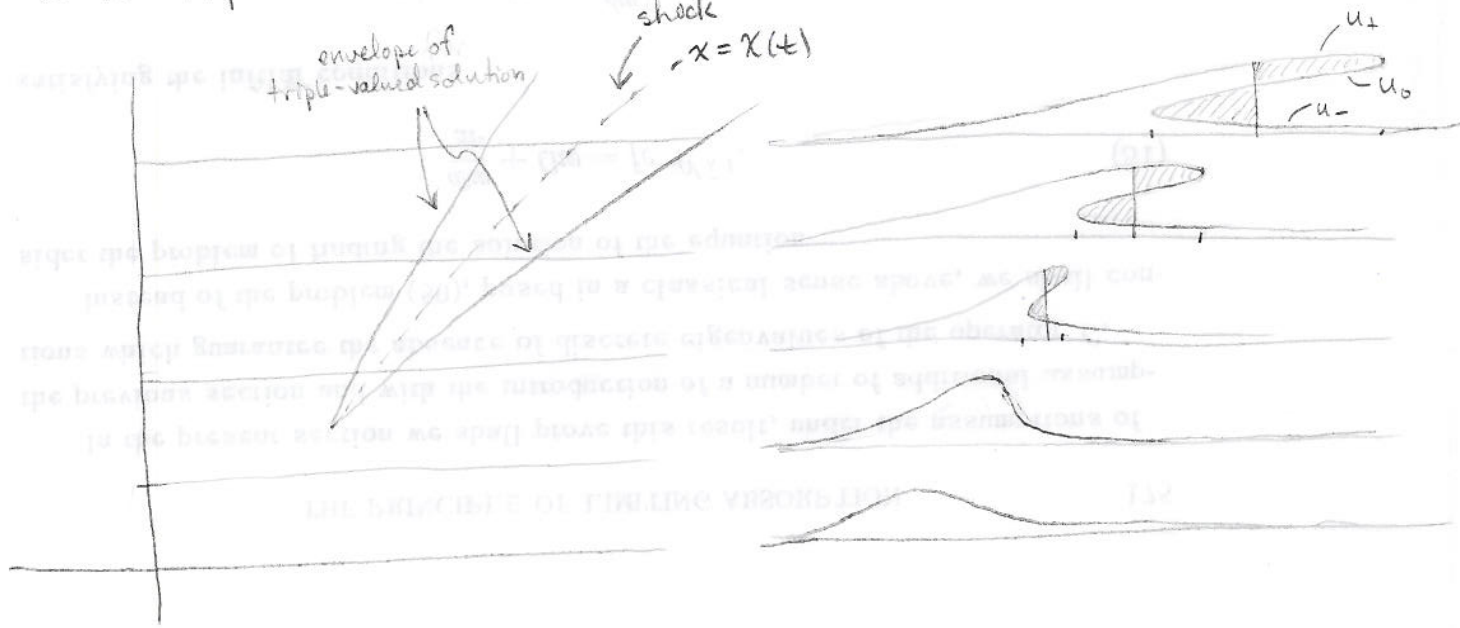
and together with $\xi_t + G(\xi)\xi_x = 0$ and $G(\xi) = c(g(\xi)) = c(u(x,t))$, this gives

$$u_t + c(u)u_x = 0 .$$

<u>Shocks</u>

When characteristic lines cross, that is, when for (x,s), $\exists\ \xi_1, \xi_2, \ldots$ such that $x = \xi_1 + c(g(\xi_1))s = \xi_2 + c(g(\xi_2))s = \cdots$ the formula $u(x,t) = g(\xi)$ can be viewed as a multi-valued solution $u(x,t) = g(\xi_1) = g(\xi_2) = \cdots$

For example, when $c(u) = u$ and $g(\xi)$ has a single maximal value, there is a region of (x,t)-space in which u is triple-valued.



In a region in which u is triple-valued, let

$$u_-(x,t) < u_0(x,t) < u_+(x,t)$$

be the three solutions. By choosing $u(x,t) = u_+(x,t)$ on one side of a curve $x = X(t)$ and $u(x,t) = u_-(x,t)$ on the other side, one can form a solution in the triple-valued region minus the curve $x = X(t)$. This curve should be chosen so that $u(x,t)$ satisfies the integral form of the conservation law,

(a)
$$\frac{d}{dt}\int_a^b u + \Big(F(u(b)) - F(u(a))\Big) = 0$$

On one hand, we calculate that [Assume $u = u_+$ to the left of $X(t)$ and $u = u_-$ to the right, as in the pictures.]

(b)
$$\frac{d}{dt}\int_a^b u = \frac{d}{dt}\int_a^{X(t)} u + \frac{d}{dt}\int_{X(t)}^b u =$$
$$= \int_a^{X(t)} u_t + \int_{X(t)}^b u_t + \Big(u_+(X(t)) - u_-(X(t))\Big) X'(t).$$

On the other hand, because u is C^1 off of $x = X(t)$,

(c)
$$\int_a^b u_t = \int_a^{X(t)} u_t + \int_{X(t)}^b u_t = F(u(a)) - F(u(b)) - \Big(F(u_+(X(t))) - F(u_-(X(t)))\Big)$$

Putting (a), (b), and (c) together yields

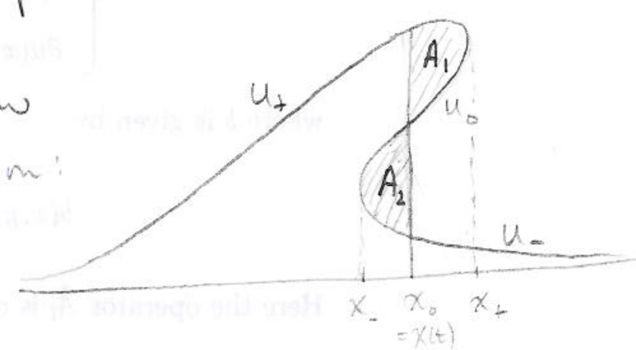
(d)
$$\Big(u_+(X(t)) - u_-(X(t))\Big) X'(t) - \Big(F(u_+(X(t))) - F(u_-(X(t)))\Big) = 0$$

or

$$X'(t) = \frac{F(u_+(X(t))) - F(u_-(X(t)))}{u_+(X(t)) - u_-(X(t))},$$

which is a differential equation for $X(t)$.

The placement of the shock, $x = X(t)$, can be understood graphically by the "rule of equal areas"; namely, the two shaded regions in the figure are of equal area.



To see this, use the conservation law applied to each branch of the solution:

$$A_1 - A_2 = \int_{x_0}^{x_+} u_+ - \int_{x_-}^{x_+} u_0 + \int_{x_-}^{x_0} u_-$$

$$\frac{d}{dt}(A_1 - A_2) = F(u_+(x_0)) - F(u_+(x_+)) - F(u_0(x_-)) + F(u_0(x_+)) + F(u_-(x_-)) - F(u_-(x_0)) +$$
$$+ u_+(x_+)\dot{x}_+ - u_+(x_0)\dot{x}_0 - u_0(x_+)\dot{x}_+ + u_0(x_-)\dot{x}_- + u_-(x_0)\dot{x}_0 - u_-(x_-)\dot{x}_-$$

Using that $u_+(x_+) = u_0(x_+)$ and $u_-(x_-) = u_0(x_-)$, this reduces to the left-hand side of (d). Thus $A_1 - A_2$ is constant in time, and since it vanishes at the initiation of the shock, it is zero for all time.

Two further references on shocks:

J. Billingham and A.C. King, Wave Motion, Cambridge U. Press, 2000.

G.B. Whitham, Linear and Nonlinear Waves, Wiley-Interscience, 1973.