

Tsinghua-Princeton-CI Summer School
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Lectures on
Dynamics of Combustion Waves
in Premixed Gases

Professor Paul Clavin
Aix-Marseille Université
ECM & CNRS (IRPHE)

Lecture III
Thermal propagation of flames

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Lecture 3: **Thermal propagation**

- 3-1. Quasi-isobaric approximation (Low Mach number)
- 3-2. One-step irreversible reaction
- 3-3. Unity Lewis number and large activation energy
- 3-4. Zeldovich & Frank-Kamenetskii asymptotic analysis

Preheated zone

Inner reaction layer

Matched asymptotic solution

- 3-5. Reaction diffusion waves

Phase space

Selected solution in an unstable medium

III – 1) Quasi-isobaric approximation. LowMach number

$$\begin{aligned} \rho(\mathbf{u} \cdot \nabla)\mathbf{u} &\approx -\nabla p \quad \Rightarrow \quad \delta p \approx \rho u \delta u \\ p &\approx \rho a^2 \quad \Rightarrow \quad \delta p/p \approx u^2/a^2 \equiv M^2 \end{aligned}$$

slow evolution $\quad \quad \quad \partial/\partial t \approx \mathbf{u} \cdot \nabla \ll a |\nabla|$

+ very subsonic flow $\quad M^2 \ll 1 \quad \Rightarrow \quad \delta p/p \ll \delta T/T = O(1)$

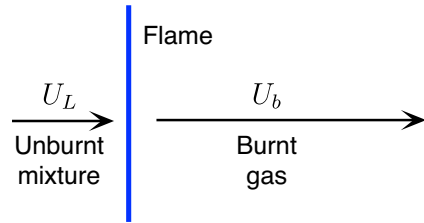
$$\begin{aligned} \frac{p}{\rho c_p T} &= O(1) \\ \left| \frac{1}{p} \frac{Dp}{Dt} \right| &\ll \left| \frac{1}{T} \frac{DT}{Dt} \right| \quad \Rightarrow \quad \left| \frac{Dp}{Dt} \right| \ll \left| \rho c_p \frac{DT}{Dt} \right| \end{aligned}$$

$$\rho c_p DT/Dt = \cancel{Dp/Dt} + \nabla \cdot (\lambda \nabla T) + \sum_j Q^{(j)} \dot{W}^{(j)}$$

(in open space)

$$\begin{aligned} \rho c_p DT/Dt &= \nabla \cdot (\lambda \nabla T) + \sum_j Q^{(j)} \dot{W}^{(j)}(T, ..Y_{k..}) \\ \rho T &= \rho_o T_o \\ \rho DY_i/Dt &= \nabla \cdot (\rho D_i \nabla Y_i) + \sum_j \vartheta_i^{(j)} m_i \dot{W}^{(j)}(T, ..Y_{k..}), \end{aligned}$$

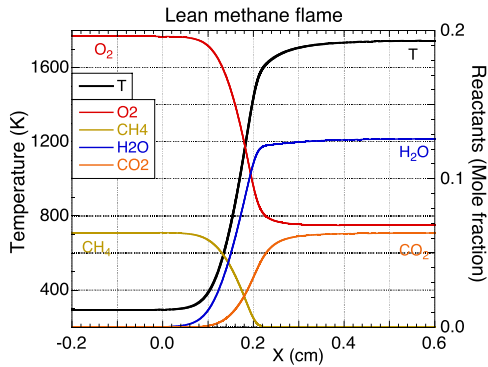
Planar flame reference frame of flame



$$\rho D/Dt = md/dx$$

$$m \equiv \rho_u U_L = \rho_b U_b, \quad U_b/U_L \approx T_b/T_u, \approx 4 - 8$$

mass flux across the planar flame



equations

$$m c_p \frac{dT}{dx} - \frac{d}{dx} \left(\lambda \frac{dT}{dx} \right) = \sum_j Q^{(j)} \dot{W}^{(j)}(T, ..Y_i..)$$

$$m \frac{dY_i}{dx} - \frac{d}{dx} \left(\rho D_i \frac{dY_i}{dx} \right) = \sum_j \nu_i^{(j)} M_i \dot{W}^{(j)}(T, ..Y_i'..),$$

m?

boundary conditions

$$x = -\infty : T = T_u, \quad Y_i = Y_{iu}, \quad \dot{W}_j = 0 \quad \text{frozen state}$$

$$x = +\infty : dT/dx = 0, \quad Y_i = Y_{ib}, \quad \dot{W}_j = 0 \quad \text{equilibrium state}$$

III – 2) One-step irreversible reaction



R in an inert ; Y = mass fraction of R

Velocity and structure of the planar flame

$$m c_p \frac{dT}{dx} - \frac{d}{dx} \left(\lambda \frac{dT}{dx} \right) = \rho q_R \dot{W} \quad q_R = \text{energy released per unit of mass of R}$$

$$m \frac{dY}{dx} - \frac{d}{dx} \left(\rho D \frac{dY}{dx} \right) = -\rho \dot{W} \quad m \equiv \rho_u U_L \text{ unknown}$$

$$x \rightarrow -\infty : Y = Y_u, T = T_u$$

$$x \rightarrow +\infty : Y = 0$$

$$m Y_u = \int_{-\infty}^{+\infty} \rho \dot{W} dx$$

$$c_p (T_b - T_u) = q_m \equiv q_R Y_u$$

Arrhenius law

$$\rho \dot{W} = \rho_b \frac{Y}{\tau_r(T)}$$

$$\frac{1}{\tau_r(T)} \equiv \frac{e^{-E/k_B T}}{\tau_{coll}}$$

$$\frac{1}{\tau_{rb}} \equiv \frac{e^{-E/k_B T_b}}{\tau_{coll}}$$

$$\frac{1}{\tau_r(T)} = \frac{1}{\tau_{rb}} e^{-\frac{T_b}{T} \beta (1-\theta)}$$

$$\beta \equiv \frac{E}{k_B T_b} \left(1 - \frac{T_u}{T_b} \right)$$

$$\theta \equiv \frac{T - T_u}{T_b - T_u} \in [0, 1]$$

III – 3) Unity Lewis number and large activation energy

$Le \equiv D_T/D$ Reduced temperature and mass fraction

$$\theta \equiv \frac{T - T_u}{T_b - T_u} \in [0, 1] \quad \psi \equiv \frac{Y}{Y_u} \in [0, 1]$$

$$m \frac{d\theta}{dx} - \rho D_T \frac{d^2\theta}{dx^2} = \rho \frac{\dot{W}}{Y_{1u}}, \quad m \frac{d\psi}{dx} - \frac{\rho D_T}{Le} \frac{d^2\psi}{dx^2} = -\rho \frac{\dot{W}}{Y_{1u}}, \quad \rho \frac{\dot{W}}{Y_u} = \rho_b \frac{\psi}{\tau_{rb}} e^{-\frac{T_b}{T} \beta(1-\theta)}$$

$$x = -\infty : \theta = 0, \psi = 1, \quad x = +\infty : \theta = 1, \psi = 0$$

$$\beta \equiv \frac{E}{k_B T_b} \left(1 - \frac{T_u}{T_b} \right)$$

$$Le = 1$$

$$\psi = 1 - \theta \quad m \frac{d\theta}{dx} - \rho D_T \frac{d^2\theta}{dx^2} = \rho \frac{\dot{W}}{Y_{1u}}, \quad \rho \frac{\dot{W}}{Y_u} = \rho_b \frac{(1-\theta)}{\tau_{rb}} e^{-\frac{T_b}{T} \beta(1-\theta)}$$

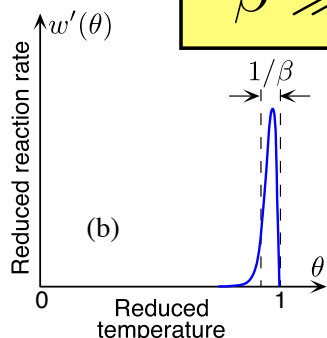
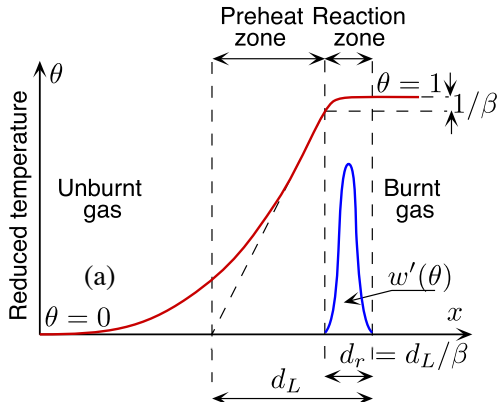
$$x = -\infty : \theta = 0, \quad x = +\infty : \theta = 1,$$

$$\beta \gg 1$$

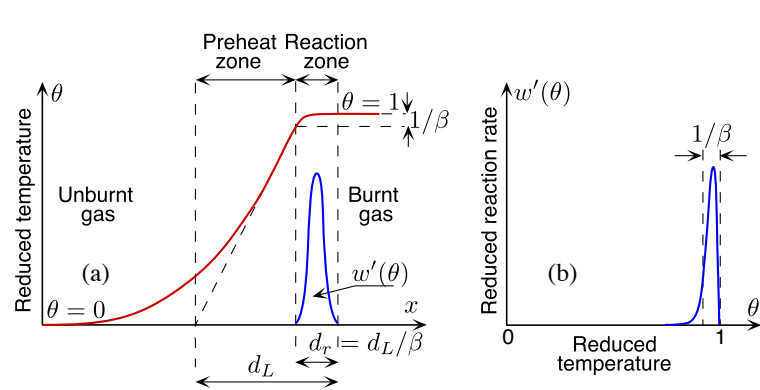
$$\rho \frac{\dot{W}}{Y_u} = \rho_b \frac{w'(\theta)}{\tau_{rb}}$$

$$w'(\theta) \approx (1-\theta) e^{-\beta(1-\theta)}$$

(reaction rate is non negligible only when $T \approx T_b$)



III – 4) Zeldovich, Frank-Kamenetskii asymptotic analysis



$$\beta \rightarrow \infty$$



Zeldovich 1938

$$m \frac{d\theta}{dx} - \rho D_T \frac{d^2\theta}{dx^2} = \rho \frac{\dot{W}}{Y_{1u}},$$

$$x = -\infty : \theta = 0, \quad x = +\infty : \theta = 1,$$

$$w'(\theta) \approx (1 - \theta)e^{-\beta(1-\theta)}$$

$$\rho \dot{W} / Y_u = \rho_b w'(\theta) / \tau_{rb}$$

preheated zone $\dot{W} \approx 0$

$$m d\theta/dx - \rho D_T d^2\theta/dx^2 = 0$$

$$\rho D_T = \text{cst.}$$

$$\theta = e^{mx/\rho D_T}$$

origin $x = 0$: location of the reaction zone $\theta = 1$

$$d_L \equiv \rho D_T / m = D_{T_u} / U_L$$

matching condition

heat flux into the preheated zone

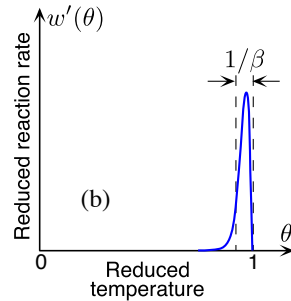
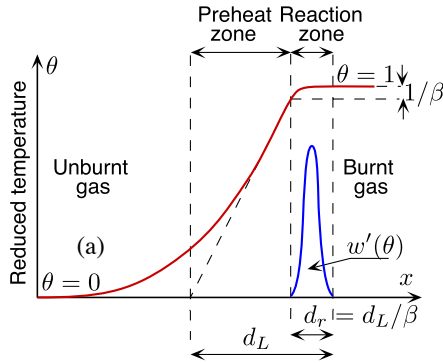
$$\rho D_T d\theta/dx|_{\theta=1} = m$$

should be equal to the heat flux from the thin reaction layer

Inner reaction layer

$$1 - \theta = O(1/\beta)$$

$$w'(\theta) \approx (1 - \theta)e^{-\beta(1-\theta)} = O(1/\beta)$$



$$\left. \begin{aligned} m \frac{d\theta}{dx} &\approx m \frac{\delta\theta}{d_r} \approx \frac{\rho_b D_{Tb}}{d_r} \frac{1}{\beta} \iff m = \rho D_T / d_L \\ \rho_b D_{Tb} \frac{d^2\theta}{dx^2} &\approx \rho_b D_{Tb} \frac{\delta\theta}{d_r^2} \approx \frac{\rho_b D_{Tb}}{d_r^2} \frac{1}{\beta} \\ \frac{\rho_b}{\tau_{rb}} w'(\theta) &\approx \frac{\rho_b}{\tau_{rb}} \delta\theta \approx \frac{\rho_b}{\tau_{rb}} \frac{1}{\beta} \end{aligned} \right\} \left. \begin{aligned} \delta\theta &= O(1/\beta) \\ d_r &\ll d_L \end{aligned} \right\} d_r \approx \sqrt{D_{Tb} \tau_{rb}}$$

~~$$m \frac{d\theta}{dx} - \rho D_T \frac{d^2\theta}{dx^2} = \frac{\rho_b}{\tau_{rb}} (1 - \theta) e^{-\beta(1-\theta)}$$~~

$$-\frac{D_{Tb}}{2} \frac{d}{dx} \left(\frac{d\theta}{dx} \right)^2 \approx \frac{1}{\tau_{rb}} (1 - \theta) e^{-\beta(1-\theta)} \frac{d\theta}{dx}$$

$$\Theta = \beta(1 - \theta) \implies \tau_{rb} \frac{D_{Tb}}{2} \left(\frac{d\theta}{dx} \right)^2 \approx \int_{\theta}^1 (1 - \theta) e^{-\beta(1-\theta)} d\theta = \frac{1}{\beta^2} \int_0^{\beta(1-\theta)} \Theta e^{-\Theta} d\Theta$$

Asymptotic solution $\beta \rightarrow \infty$ $\int_0^{\infty} \Theta e^{-\Theta} d\Theta = 1$

upstream exit of the inner layer $\beta(1 - \theta) \rightarrow \infty$: $D_{Tb} d\theta/dx \rightarrow \sqrt{(2/\beta^2) D_{Tb} / \tau_{rb}}$

downstream entrance of the external zone $\theta \rightarrow 1$: $\rho_b D_{Tb} d\theta/dx|_{\theta=1} = m$

matching

$$m = \rho_b \sqrt{(2/\beta^2) D_{Tb} / \tau_{rb}}$$

$$U_L = m / \rho_u \implies$$

$$d_r / d_L = O(1/\beta)$$



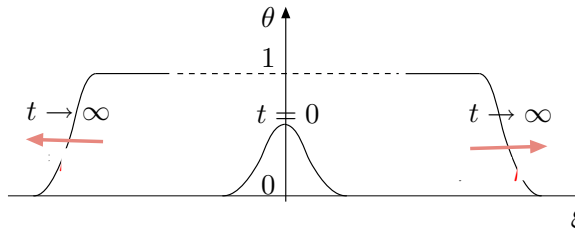
$U_L \approx \sqrt{D_{Tb} / \tau_{rb}}$
dimensional analysis

III – 5) Reaction diffusion waves

non-dimensional form $\frac{\partial \theta}{\partial t} - \frac{\partial^2 \theta}{\partial x^2} = w(\theta) \quad \theta \geq 0 \quad \theta \in [0, 1]$

propagation of steady state $\theta = 1$ into steady state $\theta = 0$

steady state: $\omega = 0$

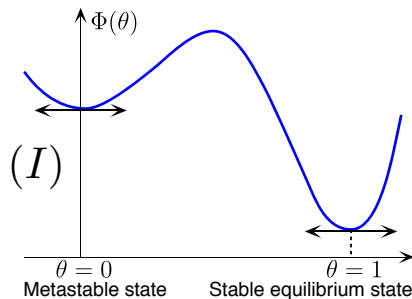


stability of steady states
 stable: $dw/d\theta < 0$,
 unstable: $dw/d\theta > 0$,

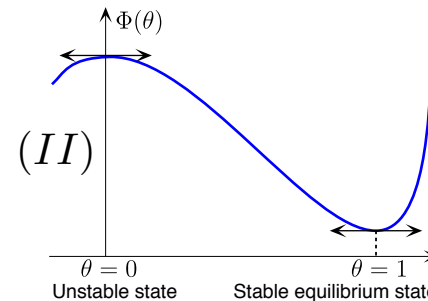
(**equilibrium** state) $\theta = 1, \quad w = 0$ **stable** steady state

two different cases depending on the property of the initial state $\theta = 0$

initial state: (I) : $\theta = 0, \quad w = 0$ **metastable** steady state (less stable)
 (II) : $\theta = 0, \quad w = 0$ **unstable** steady state (out of equilibrium)



$$d\Phi/d\theta = -w(\theta)$$



propagating planar wave at constant velocity

$$\frac{\partial \theta}{\partial t} - \frac{\partial^2 \theta}{\partial x^2} = w(\theta) \quad \text{traveling wave solution (from right to left)}$$

$$\theta \in [0, 1]$$

$$\theta(\xi)$$

$$\xi \equiv x + \mu t$$

$$\partial/\partial t = \mu d/d\xi$$

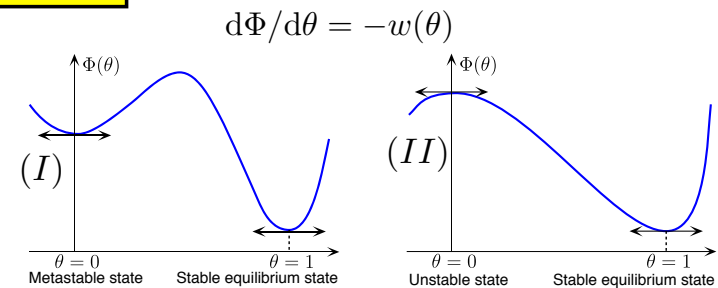
$$\partial/\partial x = d/d\xi$$

$$\mu \frac{d\theta}{d\xi} - \frac{d^2\theta}{d\xi^2} = w(\theta)$$

μ is an **eigenvalue** of the problem

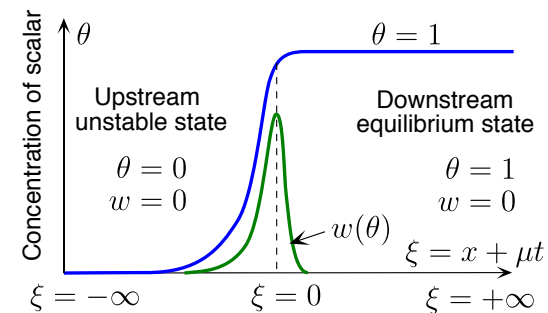
$\xi = -\infty : \theta = 0, w = 0,$
initial state

$\xi = +\infty : \theta = 1, w = 0$
final (equilibrium) state

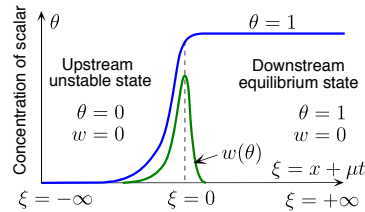


μ unknown, number of solutions ?

ZFK flame model: $\omega > 0$, case (II)



Number of solutions ? Phase space



$$\theta \geq 0$$

$$X \equiv \theta, \quad Y \equiv \mu d\theta/d\xi$$

$$dX/d\xi = Y/\mu \quad dY/d\xi = \mu [Y - \omega(X)]$$

$$\mu \frac{dX}{d\xi} - \frac{d^2X}{d\xi^2} = \omega(X) \quad \mu?$$

$$dY/dX = \mu^2 [Y - w(X)]/Y$$

Linearisation about $X = 0, Y = 0$ and $X = 1, Y = 0$

$\xi \rightarrow -\infty$ $\xi \rightarrow \infty$ (equilibrium state)

Two eigenvalues r_+ and r_- and two eigenvectors k_+ and k_-

$$\delta X = A_+ e^{\xi r_+} + A_- e^{\xi r_-}, \quad \delta Y = k_+ A_+ e^{\xi r_+} + k_- A_- e^{\xi r_-}$$

$$\mu \frac{d\delta X}{d\xi} - \frac{d^2\delta X}{d\xi^2} = \omega'_\theta \delta X$$

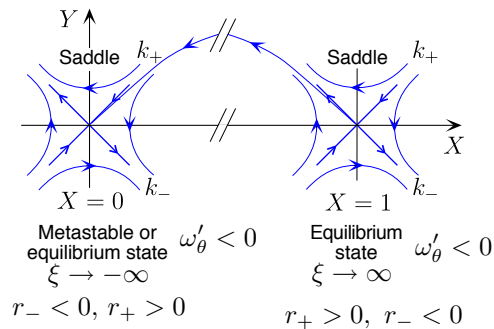
$$\mu r - r^2 - \omega'_\theta = 0$$

$$2r_\pm = \mu \pm \sqrt{\mu^2 - 4\omega'_\theta}$$

$$k_\pm = \mu r_\pm$$

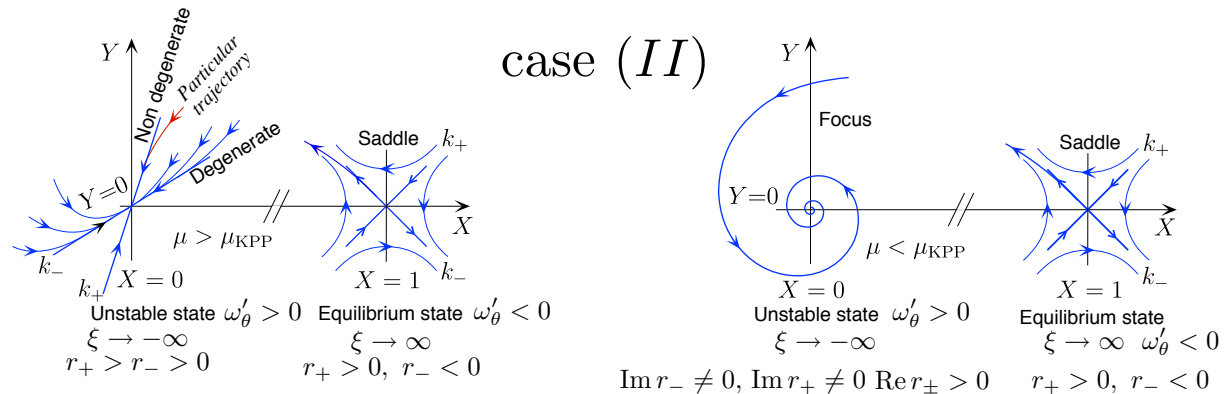
$$Y = \mu \frac{dX}{d\xi}$$

case (I)



One solution

case (II)



Infinite numbers of solutions

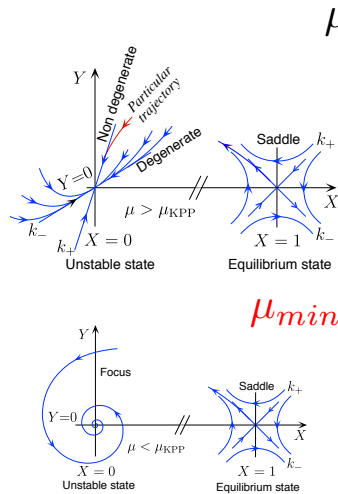
One particular solution

No solution ($\theta \geq 0$)

Unstable medium



Kolmogorov 1937



μ ↑ wave velocity

continuous spectrum with a lower bound

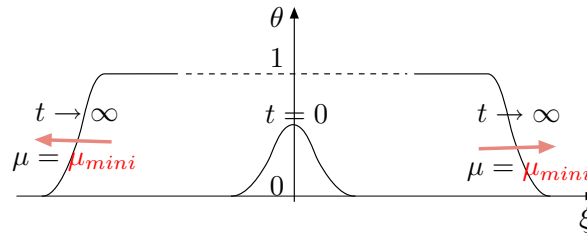
$$2r_{\pm} = \mu \pm \sqrt{\mu^2 - 4\omega'_\theta}$$

μ_{mini} soft nonlinear term $\omega(\theta)$

$$\mu_{mini} \equiv 2\sqrt{dw/d\theta|_{\theta=0}}$$

lower bound : $r_+ = r_- = \mu/2$ $k_+ = k_-$

soft case \Rightarrow collapse of the 2 eigenvalues



the lower bound solution is selected $\mu_{mini} \equiv 2\sqrt{dw/d\theta|_{\theta=0}} \neq \mu_{flame} \propto \sqrt{2 \int_0^1 w(\theta) d\theta}$

$$\partial\theta/\partial t - \partial^2\theta/\partial\xi^2 = \omega'_o\theta, \quad \text{where } \omega'_o \equiv \partial w/\partial\theta|_{\theta=0} > 0$$

$$\theta(\xi, t) \equiv Z(\xi, t)e^{+\omega'_o t} \quad \partial Z/\partial t - \partial^2 Z/\partial\xi^2 = 0$$

$$Z = e^{-\xi^2/4t}/\sqrt{t} \quad \theta \propto \exp[-\xi^2/4t + \omega'_o t - \ln(t)/2] \quad \xi^2 \approx 4\omega'_o t^2$$

OK for a soft term $\omega(\theta)$
Wrong for a stiff term $\omega(\theta)$

The lower bound solution changes of nature when $\omega(\theta)$ get stiffer

Clavin, Linan 1984

Soft $\omega(\theta) = \theta(1 - \theta)$

Stiff $w(\theta, \beta) = (\beta^2/2)\theta(1 - \theta)e^{-\beta(1-\theta)}, \beta \gg 1$