Curvature-Driven 4th-Order Diffusion from Non-Invariant Grain Boundaries.

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J. Hill, D. Arrigo, D. Triadis, W. Miller Jr., P. Vassiliou, P. Cesana

PDEs for evolution of curves and surfaces under isotropic and homogeneous processes should be invariant under Euclidean group.

Simple example is evolution by mean curvature.

Hypersurface of dimension n-1 embedded in R^n.

$$\underline{\theta} \mapsto \Re^n$$

$\hat{\mathbf{n}}$ = 'inward' unit normal vector.

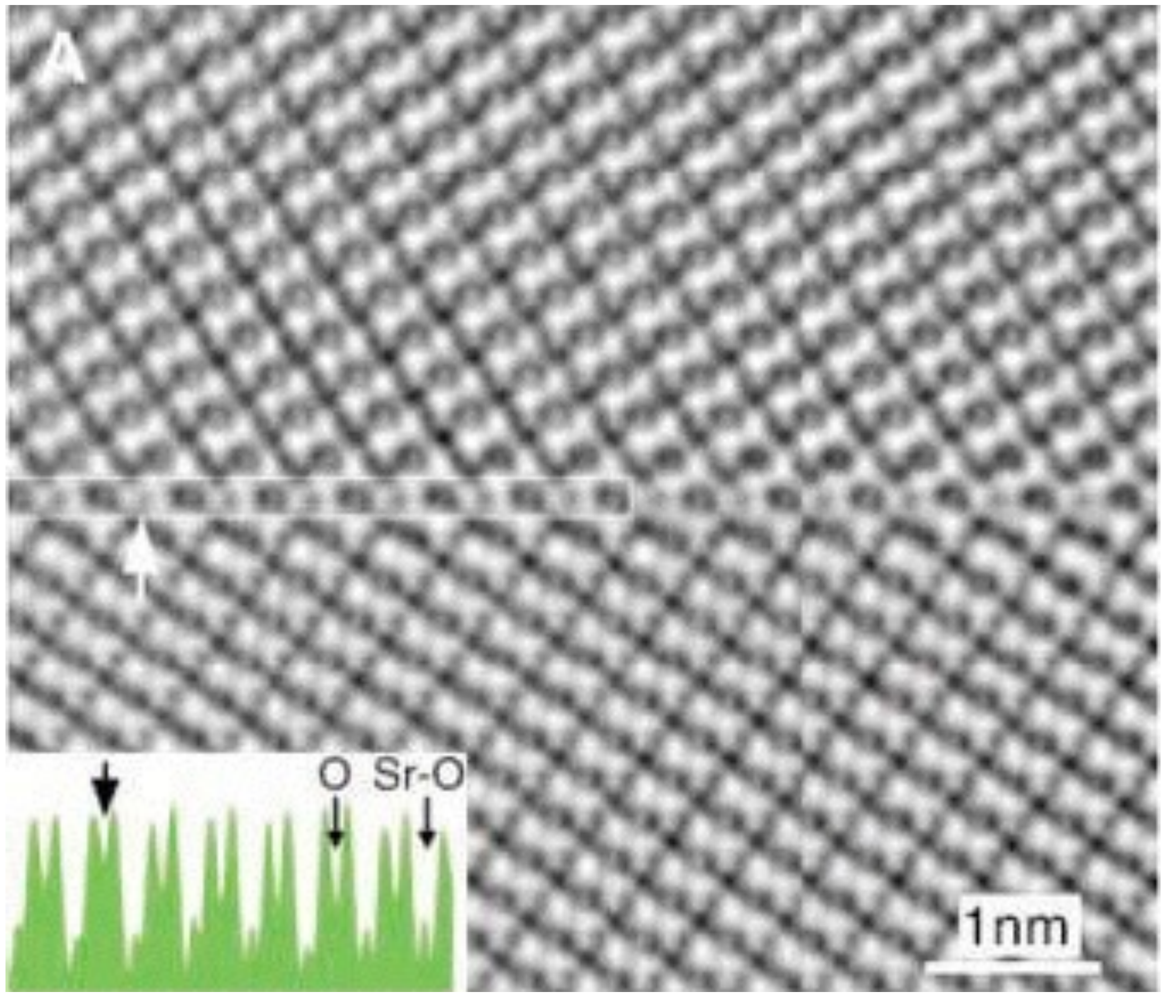
$$\hat{\mathbf{n}} \cdot \frac{\partial \mathbf{r}(\underline{\theta}, t)}{\partial t} = B\bar{\kappa}$$

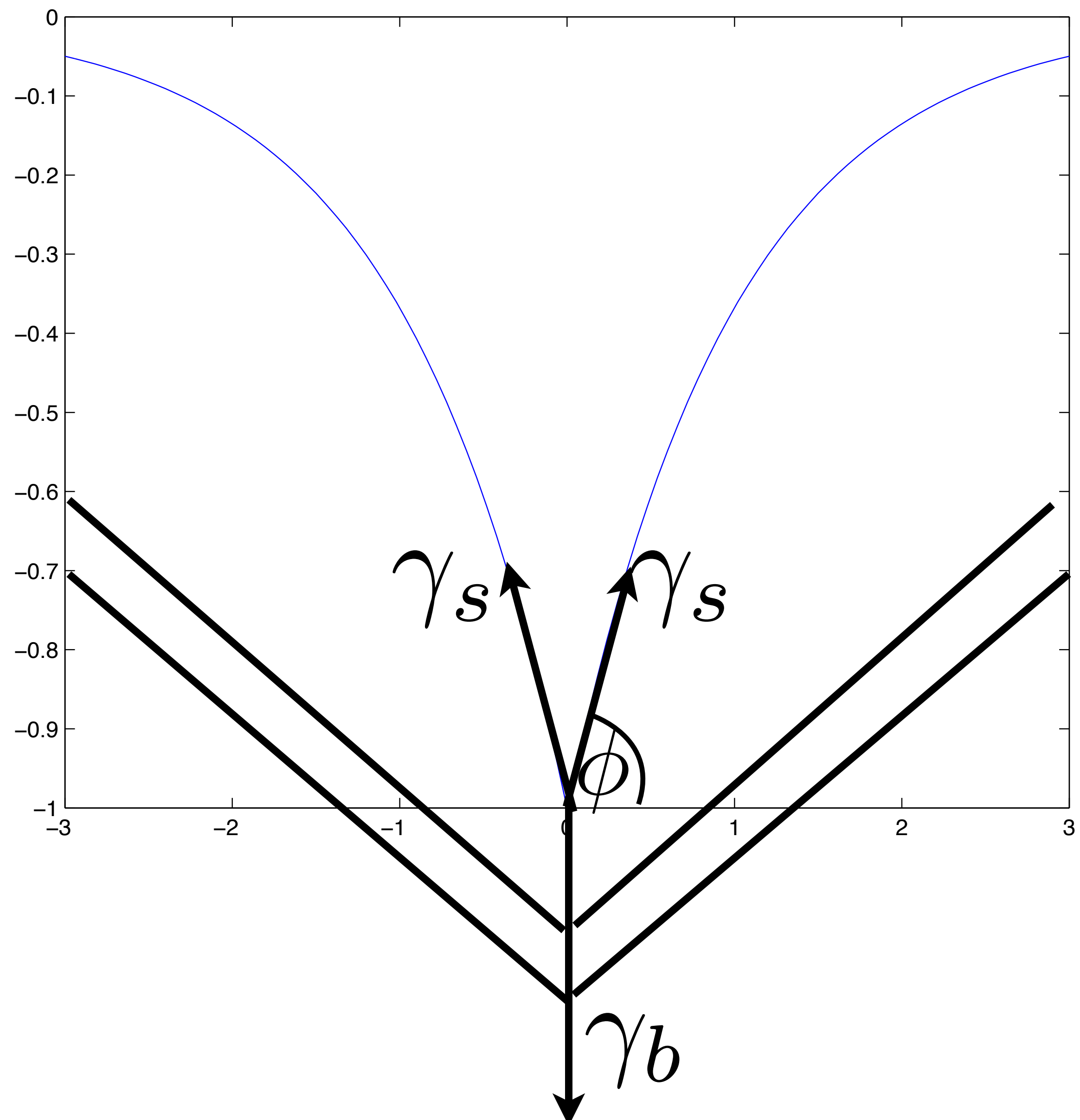
This models surface of volatile metals e.g. Mg.

Surfaces of stable metals e.g. Au, evolve by 4th order surface diffusion. In 2D,

$$\frac{\partial N}{\partial t} = -\frac{B}{2}\frac{\partial^2 \kappa}{\partial s^2}$$

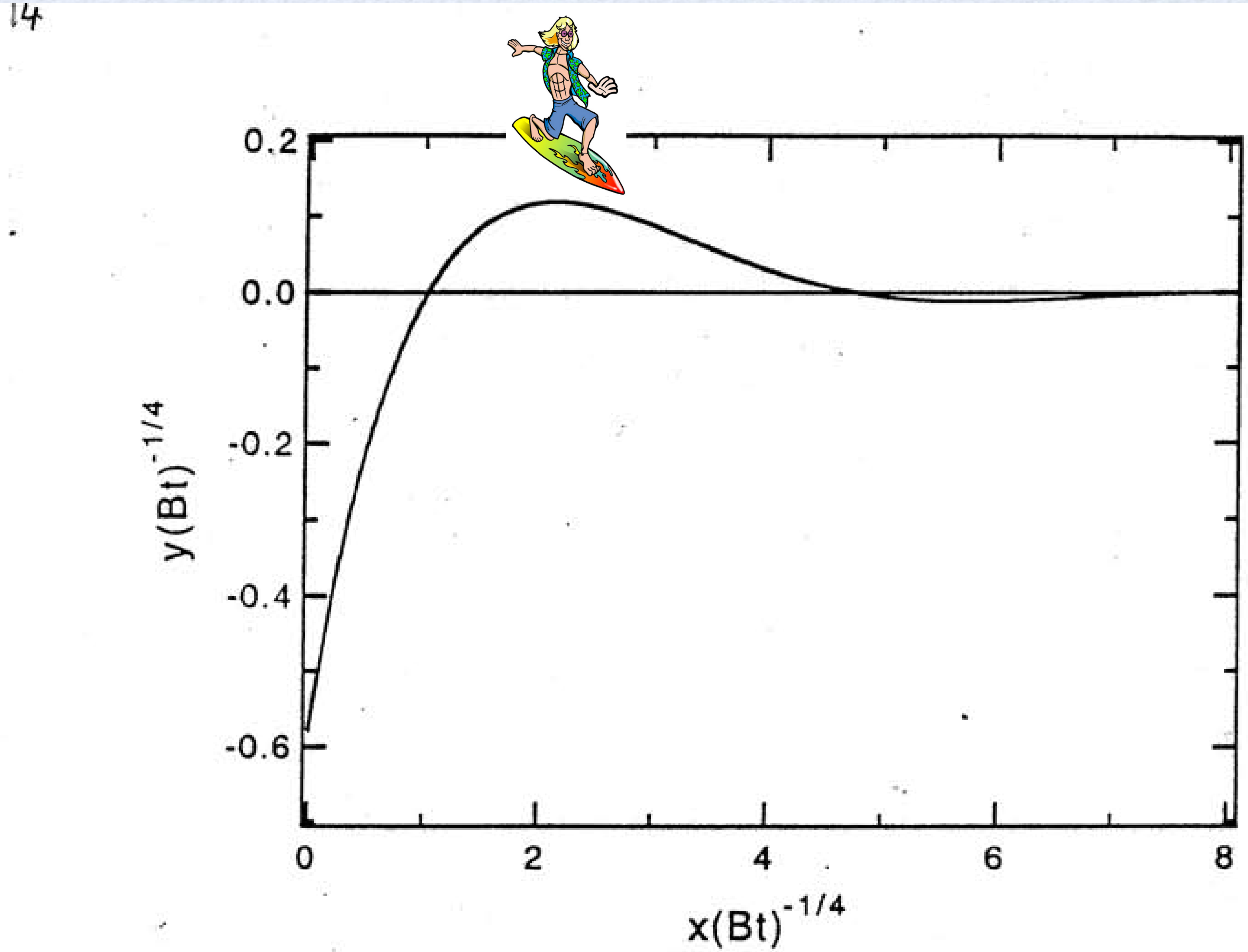
HRTEM image of grain boundary.
Z. Zhang et al, Science 302, 846-49 (2003)





$$m = tan(\phi) \; ; \; \gamma_b(T) = 2\gamma_s(T) sin(\phi)$$

Tritscher & Broadbridge, 1995



analytic solution with groove slope $y_x = 1$ at $x = 0$

Metal surface near grain boundary

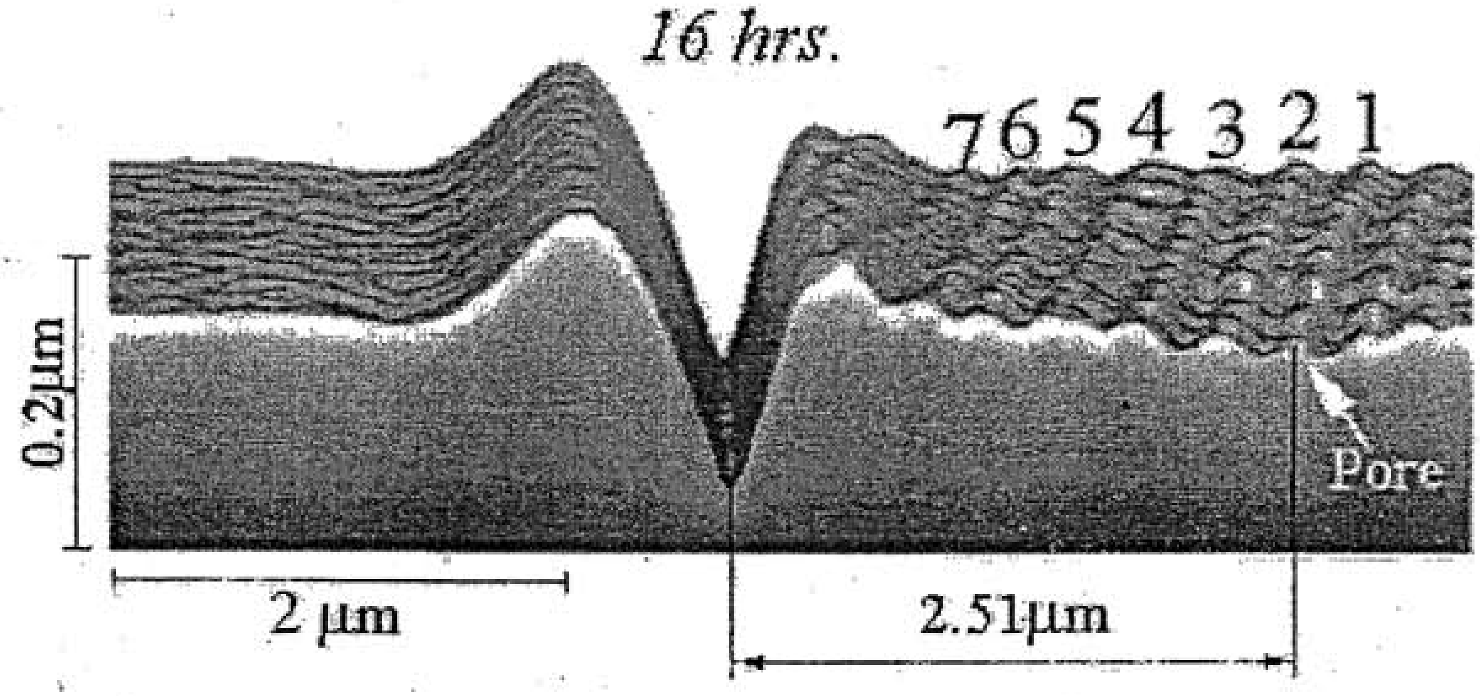


Figure 8. Three-dimensional section of the AFM image of a groove developed between unfaceted and faceted type II grain surfaces after annealing for 16h in vacuum at 1350°C. The groove is the same as that in figures 2 and 3. The front part of this section is indicated by the line in figure 3.

Sachenko, Schneibel & Zhang
Phil. Mag. A 82 (4) 815–29 (2002)

Volume flux on surface $J = \nu \Omega v$

ν = particle density

Ω = mean volume per particle

v = mean drift velocity

Nernst-Einstein Relation

$$v = \frac{-D_s}{kT} \frac{\partial \Phi}{\partial s}$$

Φ = chem pot'l per particle;

T = temp; k = Boltzmann const; D_s = surf diff const

Laplace-Herring Equation 1814 - 1950

$$\Phi = \Omega \left[\gamma_s(\phi) + \gamma_s''(\phi)\right] \kappa.$$

γ_s = surface tension

$$\phi = \arctan y_x$$

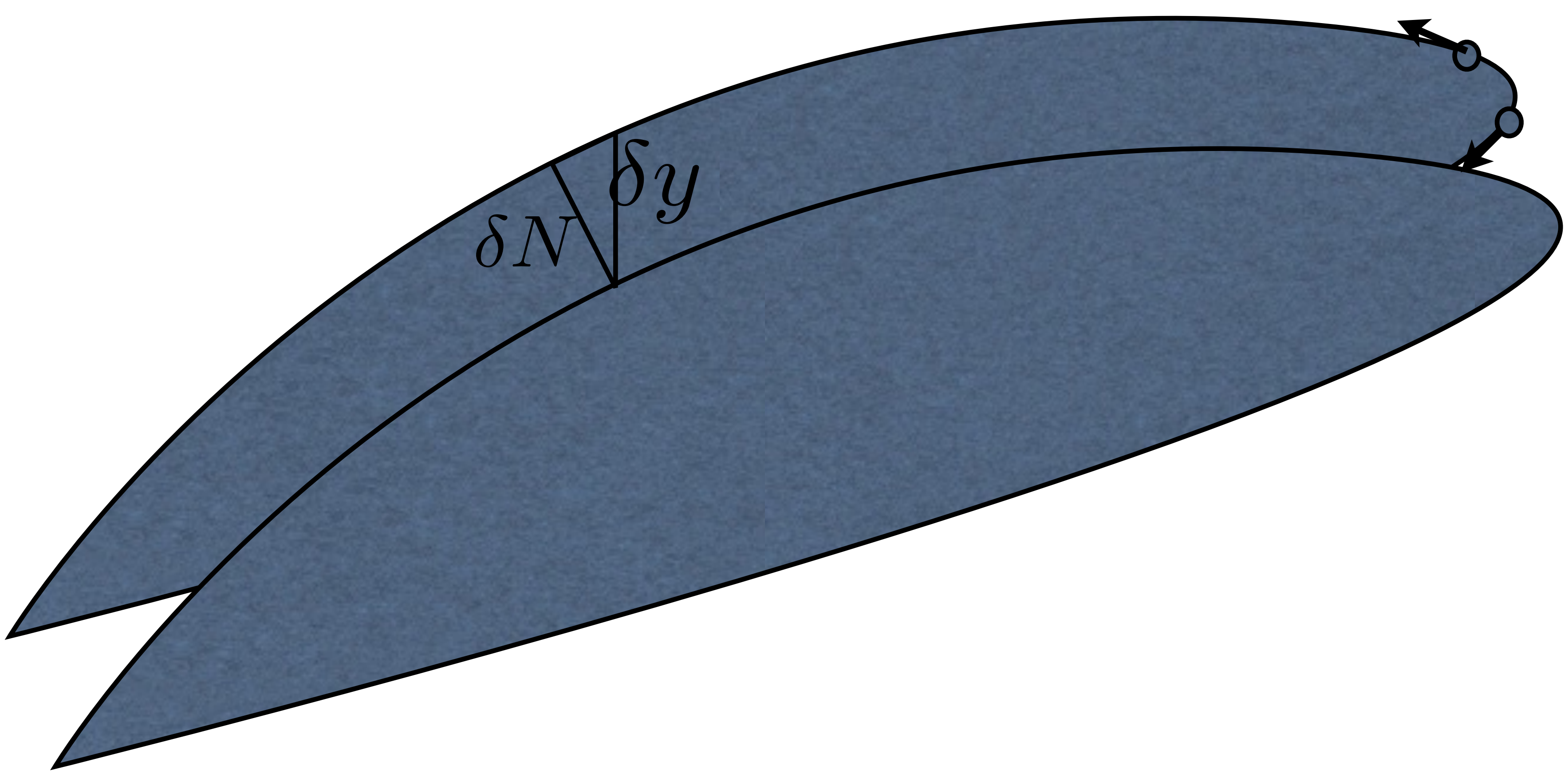
Curvature $\qquad \kappa = \dfrac{-y_{xx}}{(1+y_x^2)^{3/2}}$

Sub this flux model in local cons of mass $\quad \dfrac{\partial N}{\partial t} + \dfrac{\partial J}{\partial s} = 0$

Eq of continuity implies

$$\frac{\partial N}{\partial t} = B\frac{\partial^2 \kappa}{\partial s^2} \qquad \text{(B constant)}$$

$$cos(\phi)\frac{\partial y}{\partial t} = B\frac{\partial^2 \kappa}{\partial s^2}$$



$$\text{Now use}\quad \kappa \;=\; \left|\frac{d^2\mathbf{r}}{ds^2}\right|$$

$$= \sqrt{\left[\frac{dx}{ds}\,\frac{d}{dx}\,\frac{1}{\sqrt{1+y_x^2}}\right]^2 + \left[\frac{dx}{ds}\,\frac{d}{dx}\left(\frac{1}{\sqrt{1+y_x^2}}\,y_x\right)\right]^2}$$

$$= \; f\,(\theta)\,\theta_x\sqrt{[f'(\theta)]^2 + [\theta f'(\theta) + f\,(\theta)]^2}$$

$$\text{where } \theta = y_x\;, \quad f(\theta) = \frac{1}{\sqrt{1+\theta^2}} \;=\; \cos\phi$$

Mullins Surface Diffusion Eq + bdry conds for grooving

$$y_t = -B\,\partial_x \left\{ \left(1+y_x^2\right)^{-1/2} \partial_x \frac{y_{xx}}{\left(1+y_x^2\right)^{3/2}} \right\}$$

$$\theta_t = -B\,\partial_x^2 \left\{ f(\theta)\,\partial_x \left[\theta_x f(\theta) \sqrt{\left[f'(\theta)\right]^2 + \left[\theta f'(\theta) + f(\theta)\right]^2} \right] \right\}$$

$$y_x = \theta = m \quad , x = 0, \quad t > 0$$

$$\theta = 0 \quad , t = 0 \quad x \geq 0 \, ;$$

$$\partial_x \left[\theta_x f(\theta) \sqrt{\left[f'(\theta)\right]^2 + \left[\theta f'(\theta) + f(\theta)\right]^2} \right] = 0 \quad , \quad x = 0$$

$$\theta \to 0 \quad , \theta_x \to 0, \quad x \to \infty.$$

Anisotropic surface diffusion

in terms of rescaled dimensionless variables,

$$y_\tau = -\partial_x \left[D(y_x) \partial_x \left[E(y_x) y_{xx} \right] \right]$$

$$\tau = 0; \;\; y = 0$$

$$x \to \infty; \;\; y \to 0 \; , \;\; y_x \to 0$$

$$x = 0; \;\; J = 0 \quad \Longleftrightarrow \quad \partial_x \left[E(y_x) y_{xx} \right] = 0$$

$$x = 0 \; ; \;\; y_x = m(\tau).$$

$$m = tan(\phi) \; ; \quad \gamma_b(T) = 2\gamma_s(T) sin(\phi)$$

Surface tension $\gamma(\phi), \quad \phi = tan^{-1}\theta,$

$E \propto [\gamma''(\phi) + \gamma]/[1 + y_x^2]^{3/2}$ (Herring eq.)

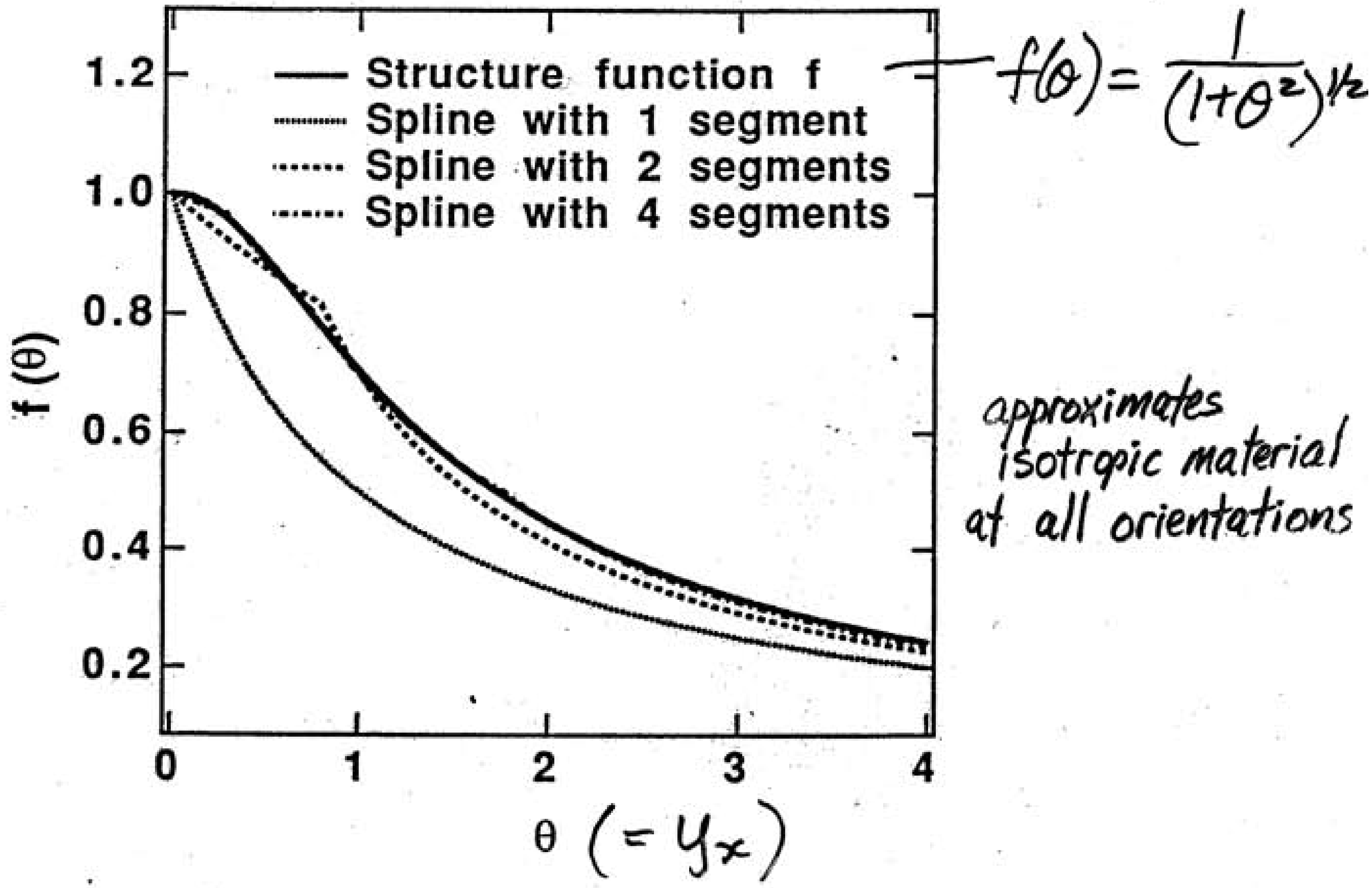
Integrable model

$$D(\theta) = \frac{\beta}{\beta + \theta}, \qquad E(\theta) = \left(\frac{\beta}{\beta + \theta}\right)^3,$$

closest to isotropic model

$$D(\theta) = \frac{1}{(1 + \theta^2)^{1/2}}, \qquad E(\theta) = \frac{1}{(1 + \theta^2)^{3/2}}$$

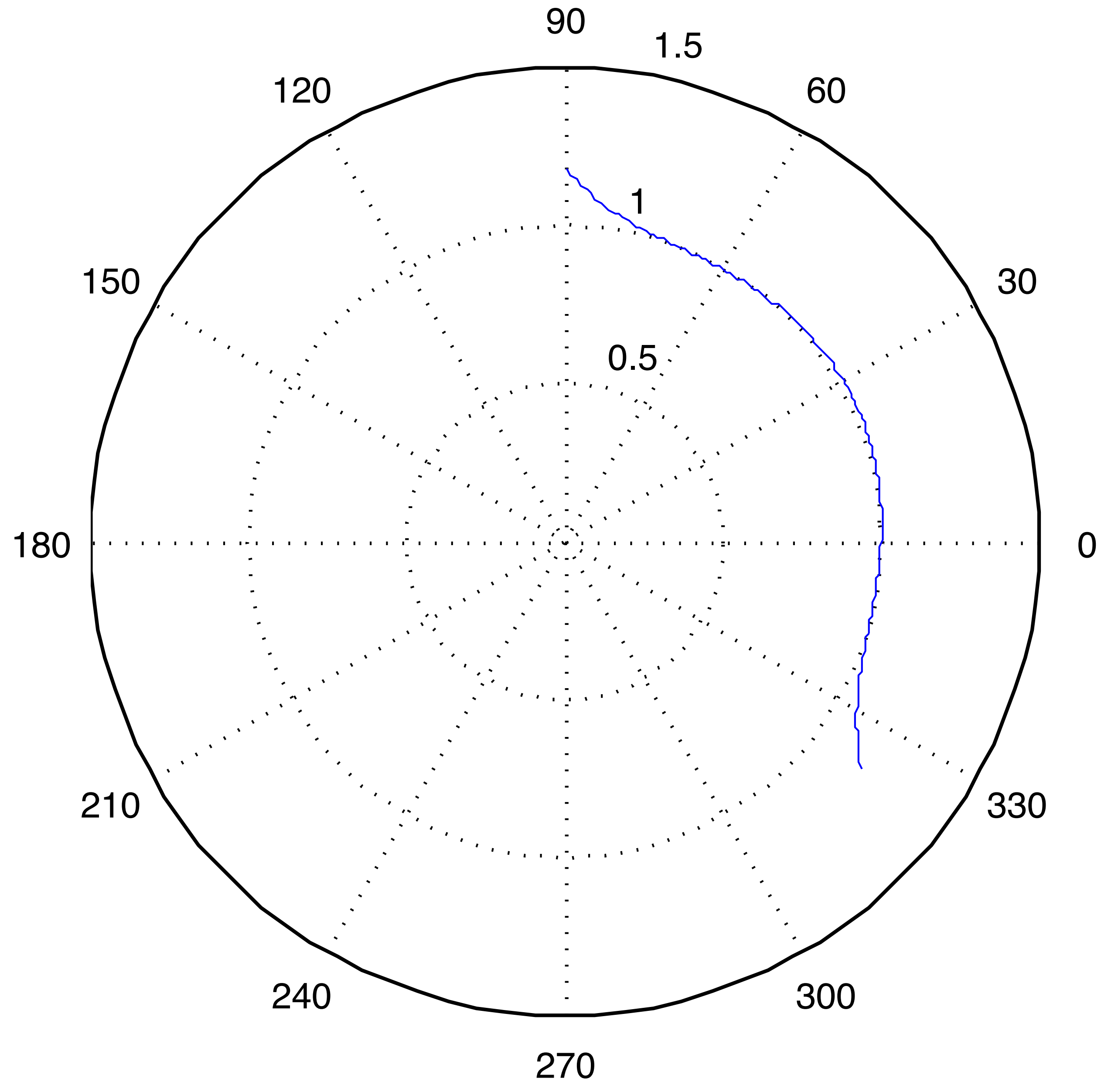
when $\beta = 2.026$



We can construct an explicit solution to Prob. II when f is piecewise inverse linear

spline f_s : $f_s(\theta) = \frac{\alpha_j}{\beta_j + \theta}$ $\quad m_{j-1} \le \theta \le m_j$

Polar plot of surface tension vs angle for integrable model



From explicit time dependence of mobility and surface tension, due to temperature change,

$$D = D_1(t)D_2(y_x); \quad E = E_1(t)E_2(y_x)\bar{\kappa}$$

, new time coordinate $\tau = \int_0^t D_1(t)E_1(t)dt$

Change of variables

$$\mu = \frac{\beta}{\beta + \theta} \qquad\qquad z = \int_0^x \frac{\beta + \theta}{\beta}\, dx$$

Transforms governing eq to linear PDE

$$\mu_\tau = -\mu_{zzzz} - \frac{1}{\beta} R(\tau) \mu_z \ ,$$

where $R(\tau) = -y_\tau(0, \tau)$.

$$\implies z = 0, \quad \mu_{zzz} = \frac{-R(\tau)}{\beta + m(\tau)}.$$

$$Z = z + \frac{1}{\beta} y(0,\tau) \quad , \mu_\tau = -\mu_{ZZZZ}$$

which has scaling symmetry

$$\bar{Z} = e^{\varepsilon} Z, \quad \bar{\tau} = e^{4\varepsilon}\tau, \quad \bar{\mu} = \mu.$$

In terms of canonical coords,

$$Y = Z\tau^{-1/4}, \quad S = log(\tau^{1/4}),$$

$$\bar{Y} = Y, \quad \bar{S} = S + \varepsilon, \quad \bar{\mu} = \mu.$$

Then separation of variables is possible

$$\mu = F(S)G(Y).$$

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$$\mu_0(Y) + \sum_{j=0}^{\infty} \tau^{j/4} \Bigg[K_{1j}\ {}_1F_3\left(\left[\frac{-j}{4}\right], \left[\frac{1}{4}, \frac{1}{2}, \frac{3}{4}\right], \frac{Y^4}{256} \right)$$

$$+K_{2j}Y\ {}_1F_3\left(\left[\frac{1}{4} - \frac{j}{4}\right], \left[\frac{1}{2}, \frac{3}{4}, \frac{5}{4}\right], \frac{Y^4}{256} \right)$$

$$+K_{3j}Y^2\ {}_1F_3\left(\left[\frac{1}{2} - \frac{j}{4}\right], \left[\frac{3}{4}, \frac{5}{4}, \frac{3}{2}\right], \frac{Y^4}{256} \right)$$

$$+K_{4j}Y^3\ {}_1F_3\left(\left[\frac{3}{4} - \frac{j}{4}\right], \left[\frac{5}{4}, \frac{3}{2}, \frac{7}{4}\right], \frac{Y^4}{256} \right) \Bigg].$$

Generalized hypergeometric function

$$ {}_1F_3([a],[b1,b2,b3],z) = \sum_{k=0}^{\infty} \frac{(a)_k}{(b1)_k (b2)_k (b3)_k} \frac{z^k}{k!} $$

$$ (a)_k = a(a+1)(a+2)\ldots(a+k-1) $$

For m const, we have similarity solution of form

$$ y\tau^{-1/4} = H(x\tau^{-1/4}) $$

For m varying with t, assume

$$ y(0,\tau) = \beta\tau^{1/4} \sum_{i=0}^{\infty} b_i \tau^{i/4} $$

These expansions for y(0,t) and μ(Z,t) can solve the free boundary problem with boundary conditions specified at unknown location

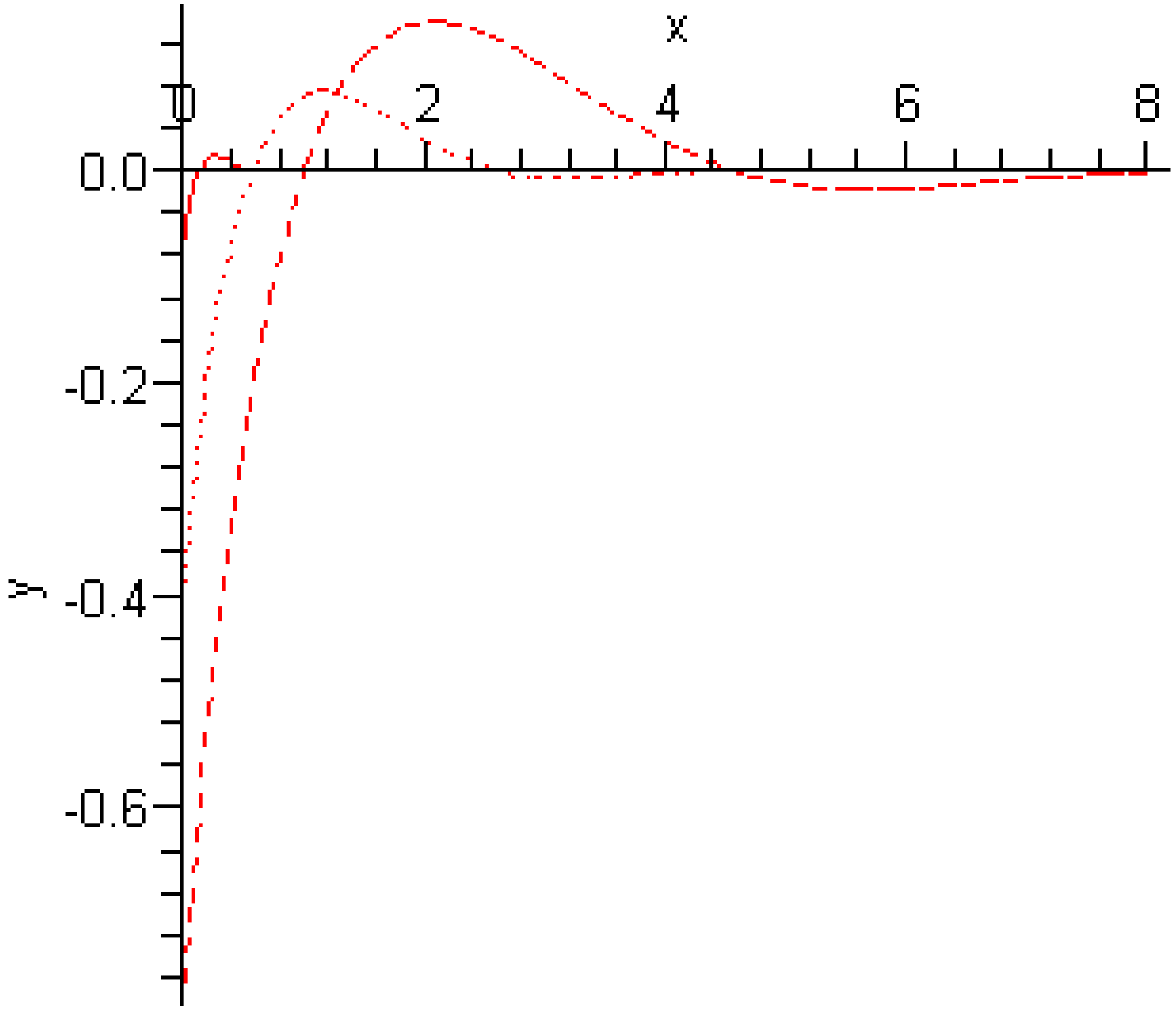
$$x = 0 \iff Z = y(0,\tau)/\beta.$$

In order to implement boundary conditions at infinity, match Laplace transform of power series solution with

$$\bar{\mu} = \exp\left(\frac{-p^{\frac{1}{4}} Z}{\sqrt{2}}\right)\left[C_3(p)\cos\left(\frac{p^{\frac{1}{4}} Z}{\sqrt{2}}\right) + C_4(p)\sin\left(\frac{p^{\frac{1}{4}} Z}{\sqrt{2}}\right)\right] + \frac{1}{p}$$

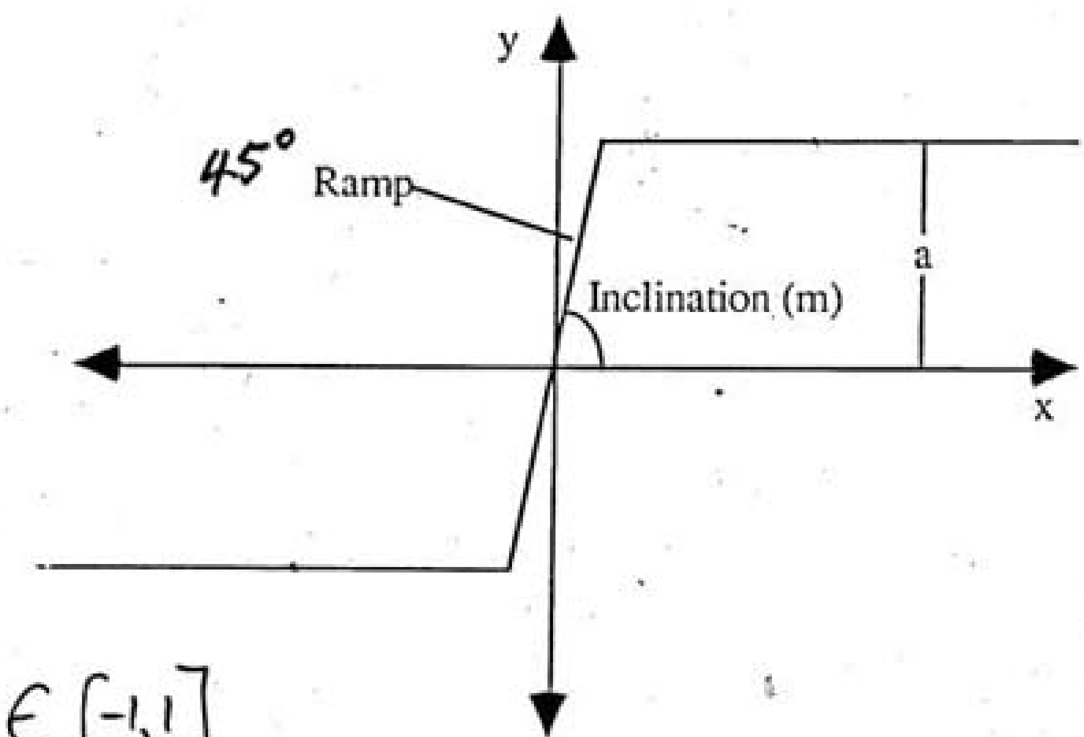
$$\bar{\mu} = \exp\left(\frac{-p^{\frac{1}{4}}Z}{\sqrt{2}}\right)\left[C_3(p)\cos\left(\frac{p^{\frac{1}{4}}Z}{\sqrt{2}}\right) + C_4(p)\sin\left(\frac{p^{\frac{1}{4}}Z}{\sqrt{2}}\right)\right] + \frac{1}{p}$$

By matching with $\mu(0,\tau)$, & $\mu_Z(0,\tau)$,
$C_3(p)$ and $C_4(p)$ can be deduced.
With j fixed, K_{1j}, K_{2j}, K_{3j} and K_{4j} are linearly dependent since they are functions of the two independent power series coefficients in $\mathcal{L}^{-1}C_3(p)$ and $\mathcal{L}^{-1}p^{1/4}C_4(p)$



$$m(\tau) = {}^{1}/_{2} + {}^{1}/_{2}\ \tau^{1/4}$$

________________ t=0.0002
..............t=0.1
----------------t=1



$y \in [-1,1]$

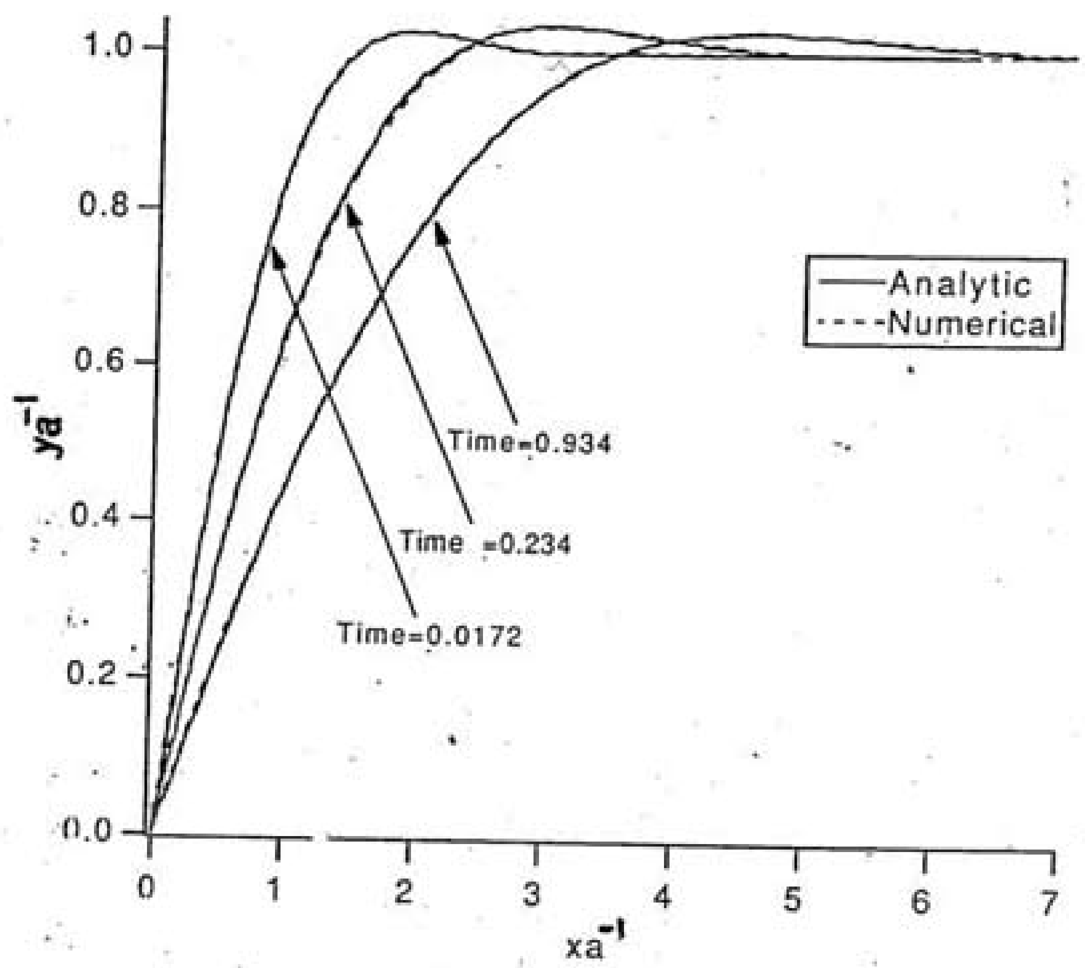
$x(y,t)$ satisfies linear P.D.E.

Use Fourier series

Use $f(\theta) = \left(\frac{\alpha}{\alpha + y_x}\right)$, not spline

Validation of numerical model (400 grid points) against analytic model with $f(y_x) = \dfrac{\alpha}{\alpha + y_x}$; $\alpha = 30$;

$\alpha = 3.07$



Note hump at top of ramp.

- effect of 4th order diffusion
- has no analogue of maximum principle.

Mullins 1957 theory of evaporation-condensation.
Lateral mixing of vapour keeps pressure close to that above flat surface. Linear model of non-equilibrium evaporation rate gives

$$-\frac{\partial N}{\partial t} = \Omega J = \frac{\Omega\alpha(p_{eq} - p)}{\sqrt{2\pi m k T}},$$ Omega being spec vol per particle.

Laplace showed that energy per unit volume of surface material is

$2\gamma_s\bar{\kappa}$ so energy platform per particle is $E = 2\Omega\gamma_s\bar{\kappa}$.

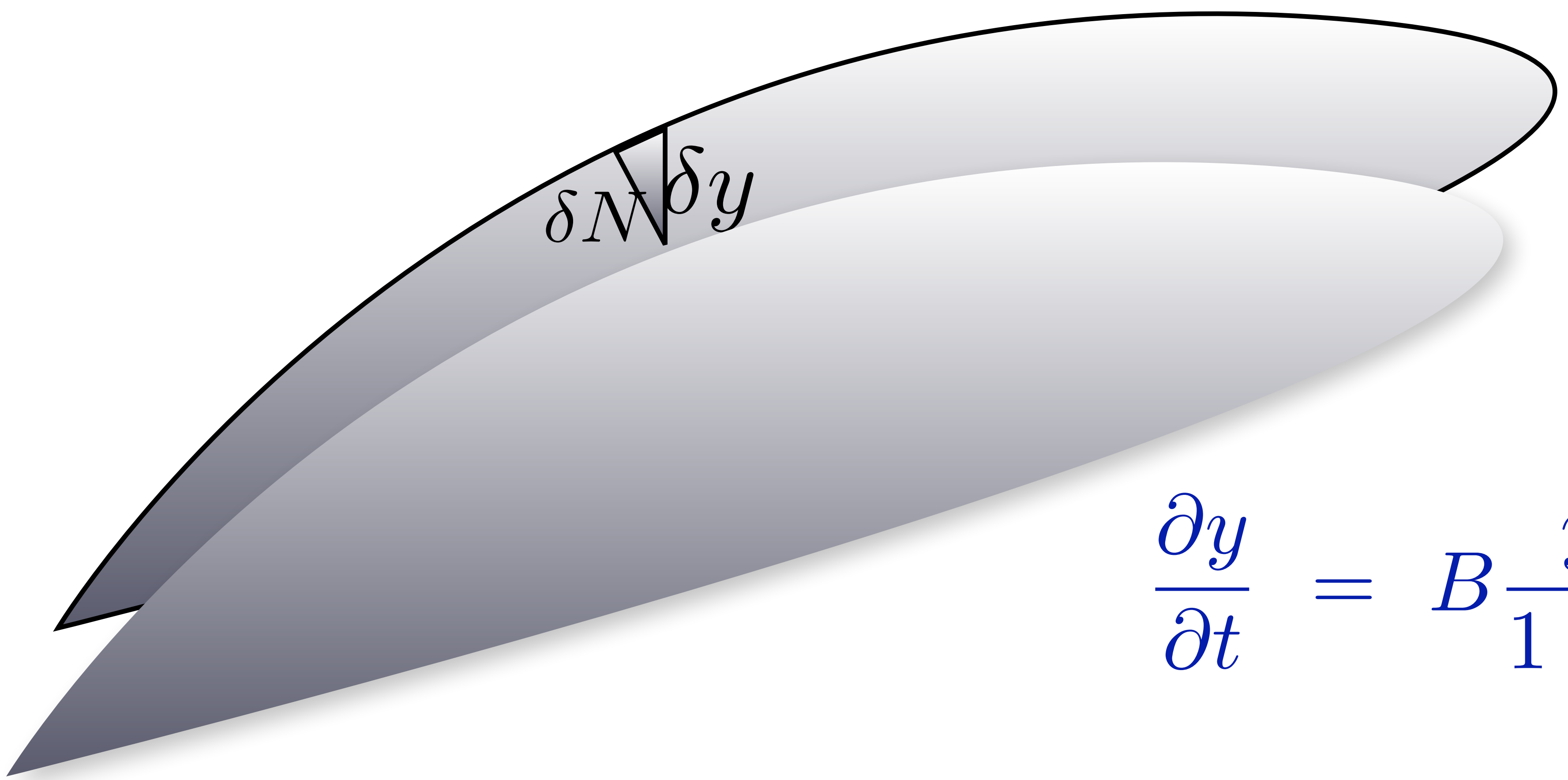
Gibbs-Thompson formula

$$p_{eq} - p = p(e^{E/kT} - 1) \approx 2p\Omega\gamma\bar{\kappa}/kT$$

implies evaporation rate proportional to mean curvature.

Around linear groove, z-direction is irrelevant.
Evaporation equation reduces to curve-shortening equation.

$$cos(\phi)\frac{\partial y}{\partial t} \;=\; \frac{1}{(1+y_x^2)^{1/2}}B\frac{y_{xx}}{1+y_x^2}$$



$$\frac{\partial y}{\partial t} \;=\; B\frac{y_{xx}}{1+y_x^2}$$

CSE in differentiated form

$$\theta_t = \partial_x[D(\theta)\theta_x] = \partial_x^2[\arctan(\theta)];\; \theta = y_x;\; D(\theta) = B/(1+\theta^2)$$

$$y_t = D(y_x)y_{xx}$$

Fujita 1952-54 presented exact similarity solutions for u(x,t) with

$$D(\theta) = \frac{1}{a\theta + b}\;,\; D(\theta) = \frac{1}{(a\theta+b)^2}\;,\; D(\theta) = \frac{1}{(a\theta+b)^2 + c}$$

Bluman and Reid 1988: these come from "potential" symmetries, or from point symmetries of the system $y_x = \theta\;;\; y_t = D(\theta)\theta_x$

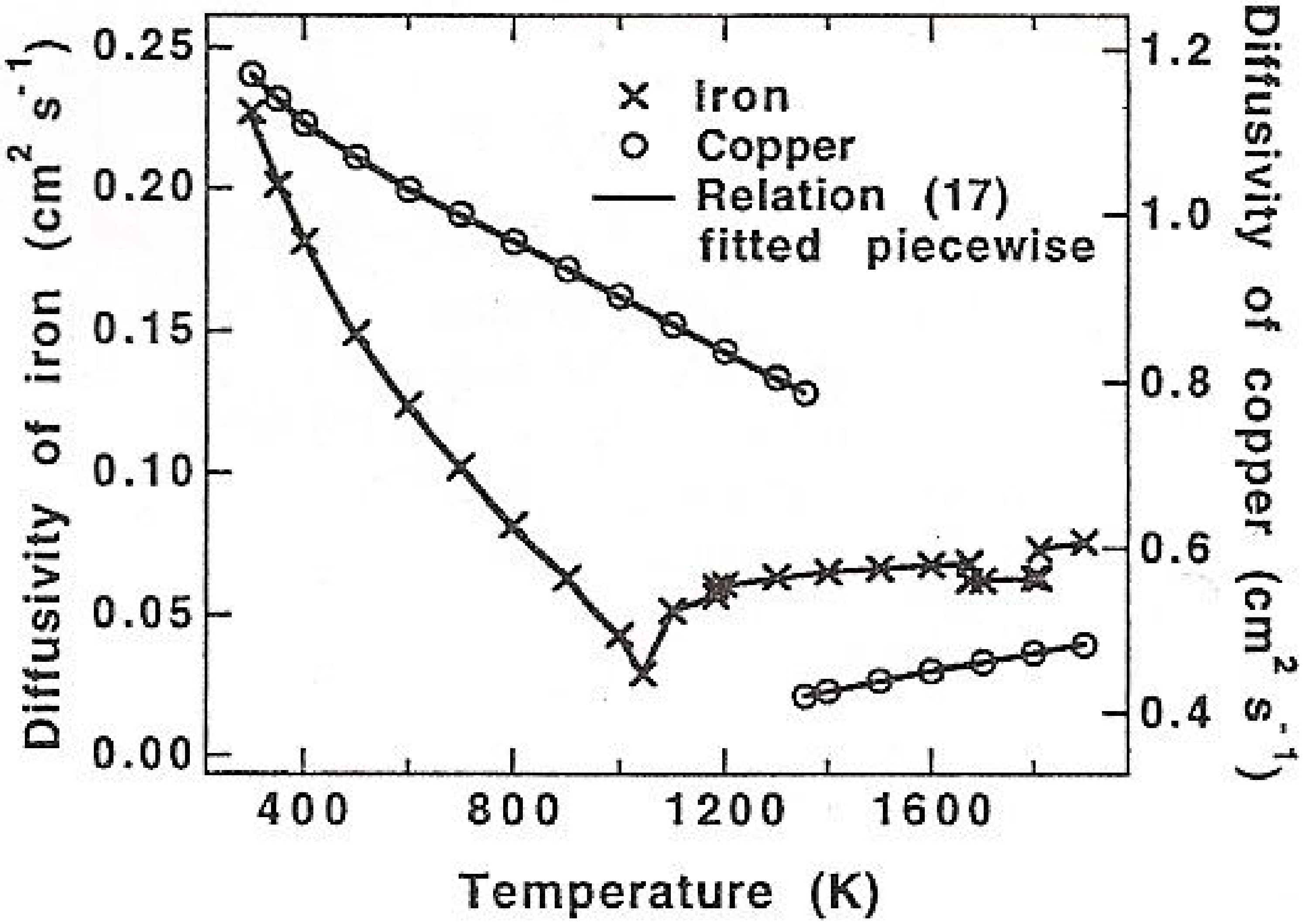


FIG. 1. Recommended thermal diffusivity of iron and copper versus temperature [27].

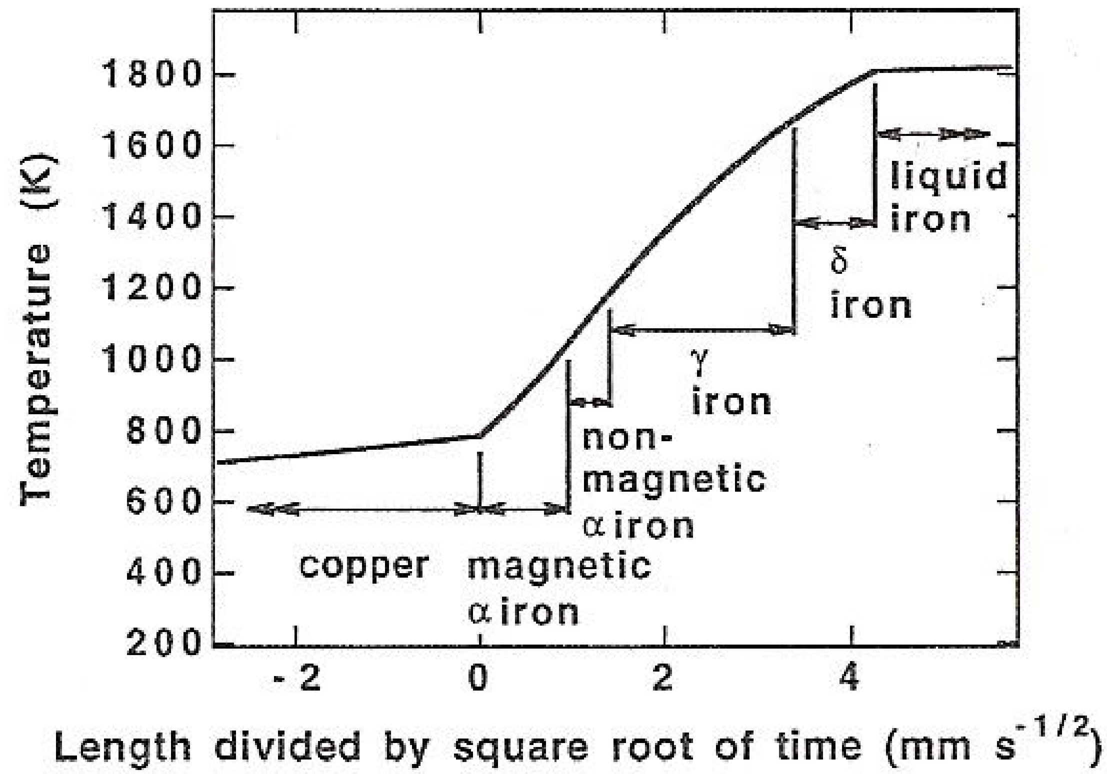


FIG. 3. Temperature distribution for the solidification of iron on a copper base. The initial temperatures were 1830 K for the iron and 300 K for the copper.

P. Tritscher & PB,
I.J. Heat Mass Transf 1994

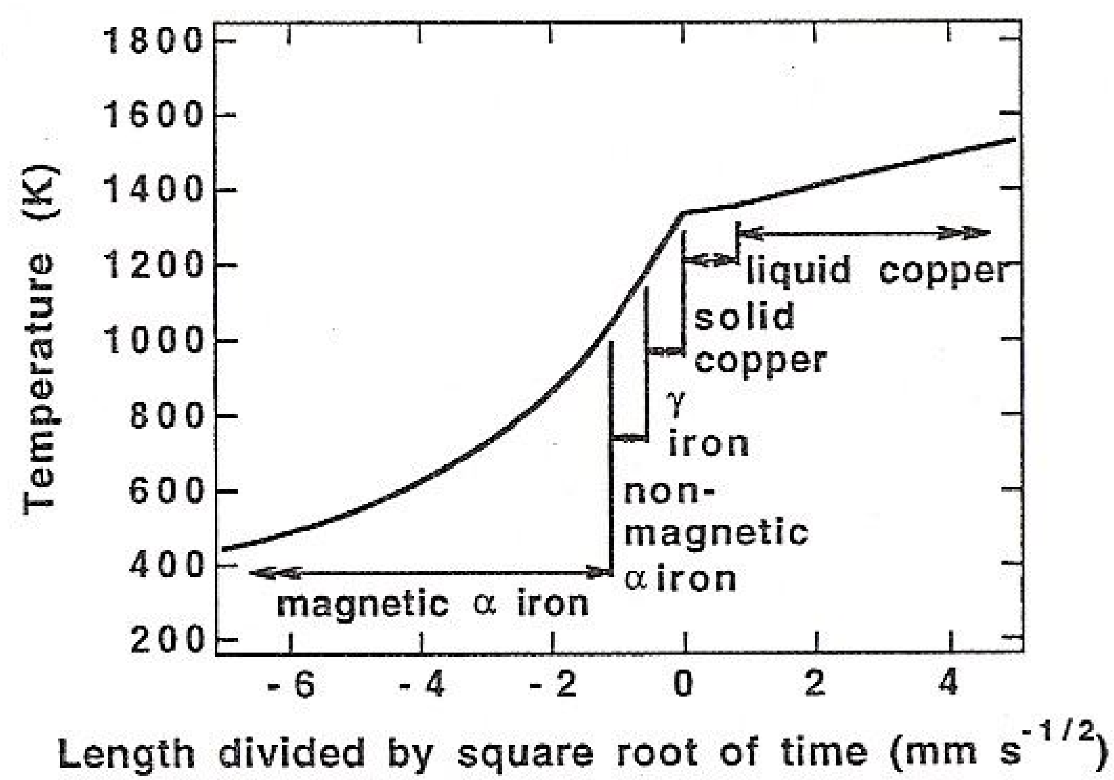


FIG. 4. Temperature distribution for the solidification of copper on an iron base. The initial temperatures were 1830 K for the copper and 300 K for the iron.

Broadbridge 1989: Exact CSE parametric similarity solution for grain boundary groove $\Theta \mapsto (\eta, \rho) = (x/2\sqrt{t}, y/2\sqrt{t})$

$$\Theta = m^{-1} tan[F(\theta;\epsilon)] \; ; \quad 0 \le \Theta \le \Theta^*$$

$$\Theta = m^{-1} tan[G(\theta;\epsilon)] \; ; \quad \Theta^* \le \Theta \le 1$$

$$\rho = m[\eta\Theta - H(\theta;\epsilon)]$$

$$\eta = \epsilon^{-1/2}\theta sin[F(\theta;\epsilon)] + (1-\theta^2-\epsilon ln\theta)^{1/2} cos[F] \; ; \; 0 \le \Theta \le \Theta^*$$

$$\eta = \epsilon^{-1/2}\theta sin[G(\theta;\epsilon)] + (1-\theta^2-\epsilon ln\theta)^{1/2} cos[G] \; ; \; \Theta^* \le \Theta \le 1$$

$$F(\theta;\epsilon) = \int_0^\theta (1-q^2-\epsilon ln q)^{-1/2} dq$$

$$G(\theta;\epsilon) = tan^{-1} m - F(\theta;\epsilon) + F(\theta_m;\epsilon)$$

$$H(\theta;\epsilon) = \epsilon^{-1/2} m^{-1} \theta \sec[F(\theta;\epsilon)] \; ; \; 0 \le \Theta \le \Theta^*$$

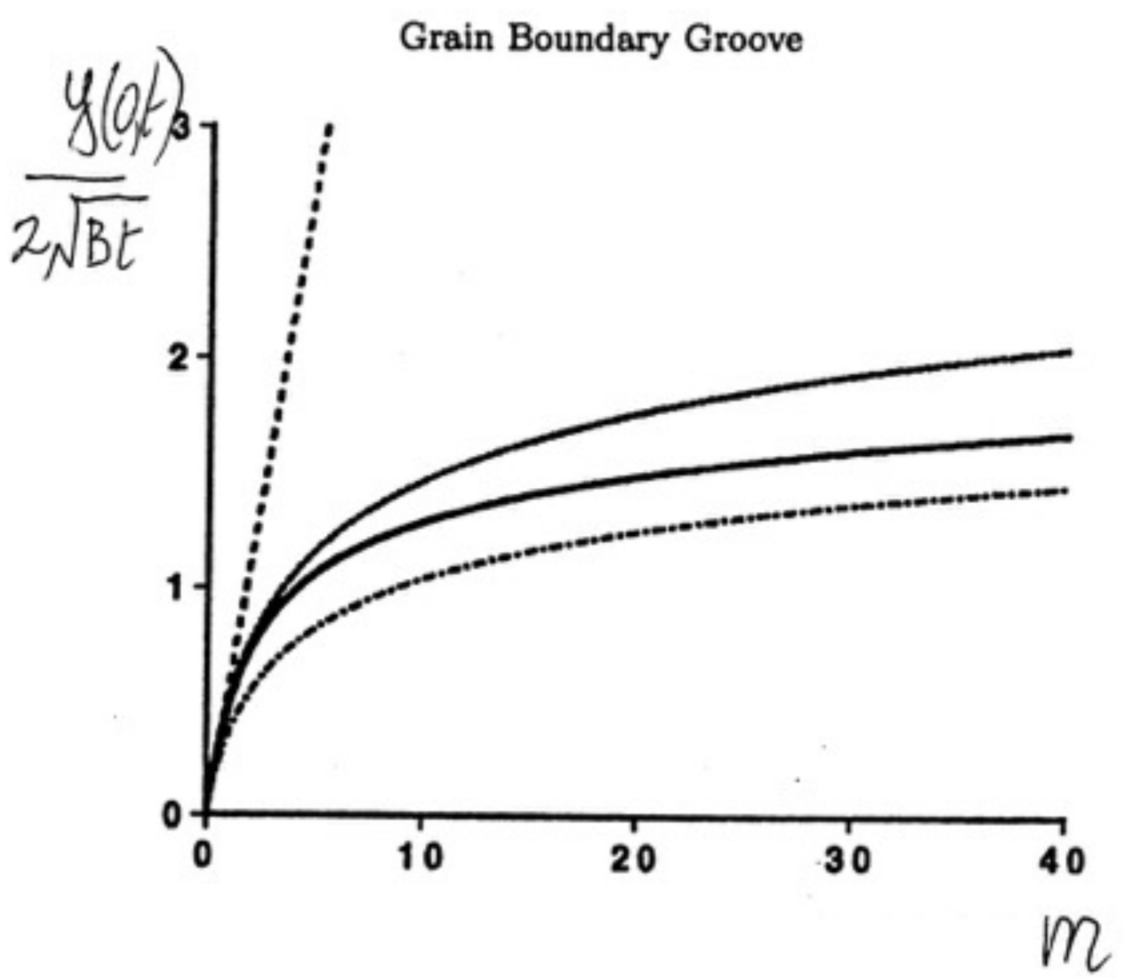
$$H(\theta;\epsilon) = \epsilon^{-1/2} m^{-1} \theta \sec[G(\theta;\epsilon)] \; ; \; \Theta^* \le \Theta \le 1$$

$$\Theta^* = m^{-1} tan[F(1;\epsilon)] \; ; \; \epsilon = \frac{\theta_m^2 - 1 - m^2}{\theta_m^2 ln \; \theta_m}$$

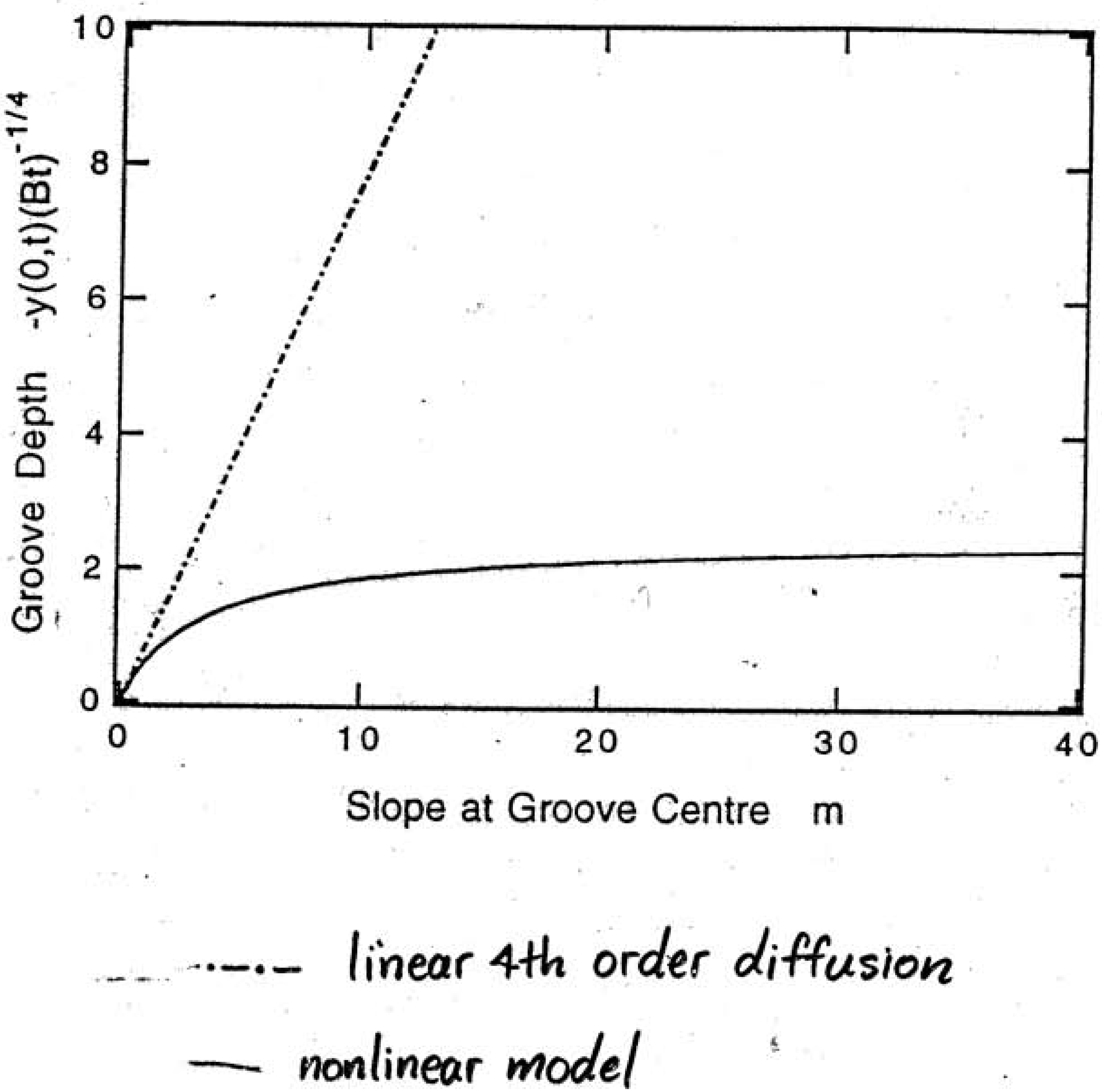
$$2F(1;\epsilon) - F(\theta_m;\epsilon) = tan^{-1} m$$

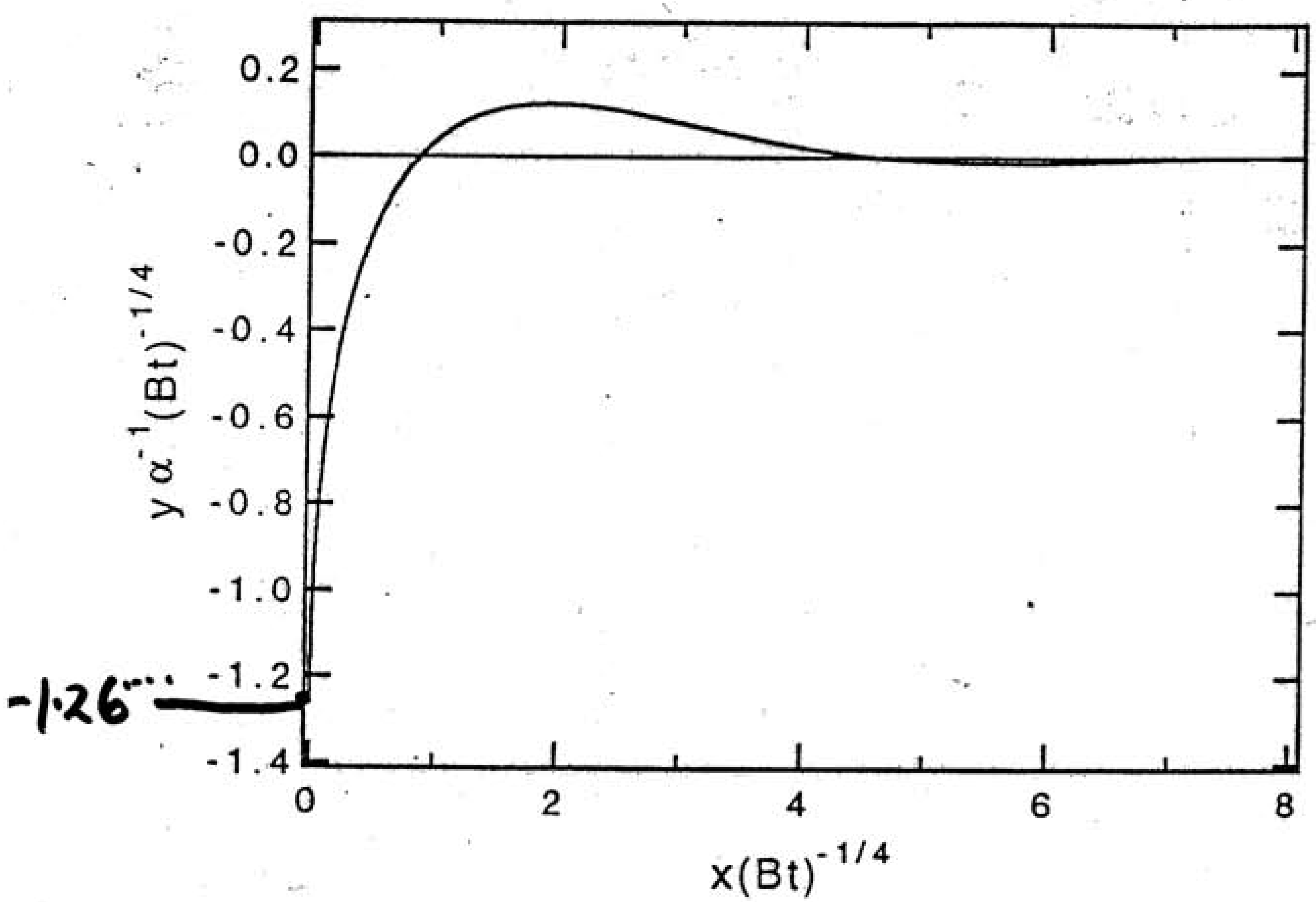
Arrigo et al 1997: for classical diffusion, groove depth F(0) proportional to m but for CSE with m sufficiently large,

$$\left(ln(\frac{m}{2\sqrt{\pi}})+\frac{1}{4}\right)^{1/2}-\frac{1}{2}\leq\frac{|y(0,t)|}{\sqrt{(Bt)}}\leq\left(2ln(\frac{m}{\sqrt{\pi}})\right)^{1/2}$$



Groove depth due to surface diffusion.





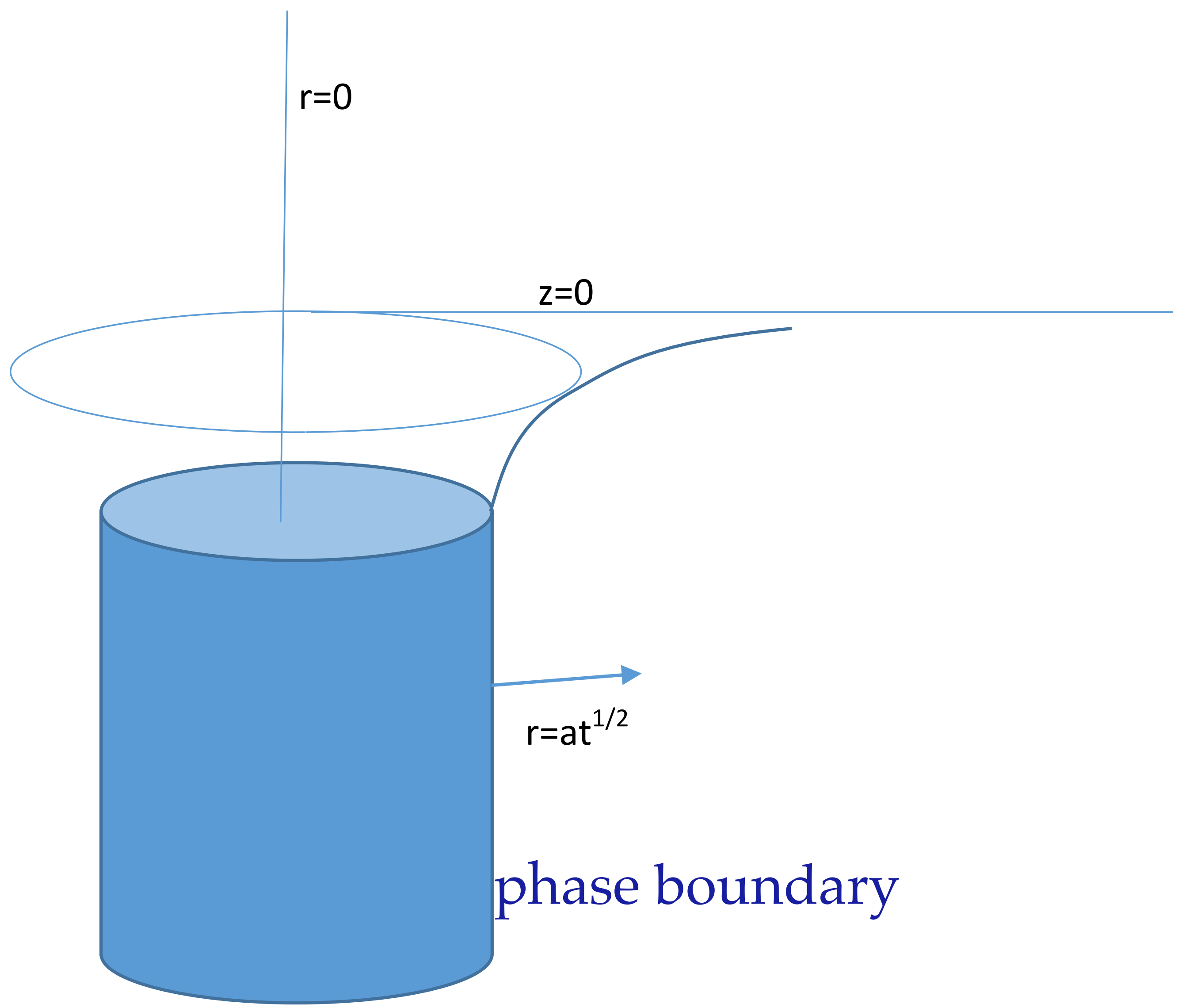
Thermal groove with infinite slope at $x=0$

Evaporation at axi-symmetric surface by mean curvature:

$$z_t = B[\frac{z_{rr}}{(1+z_r^2)^{1/2}} + \frac{1}{r} z_r]$$

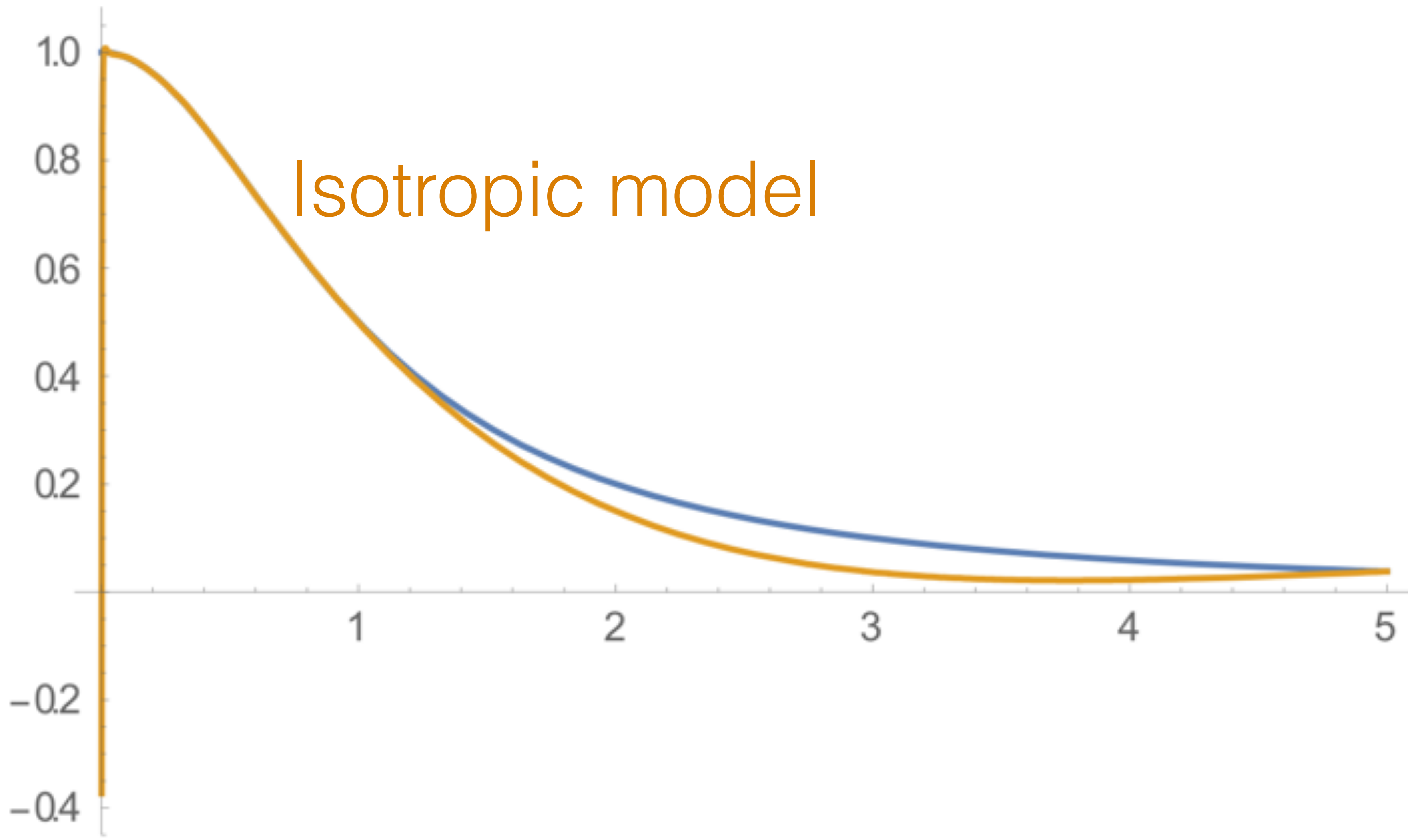
$$z_r = m, \quad r = at^{1/2}\ ; \quad z = 0,\ t = 0\ ; \quad z \to 0,\ r \to \infty$$

$$\theta = z_r; \quad \rho = rt^{-1/2}; \quad \theta = f(\rho)$$



Gallage, PB, Triadis and Cesana use inverse method previously applied to 1D nonlinear diffusion J. Philip (1960).

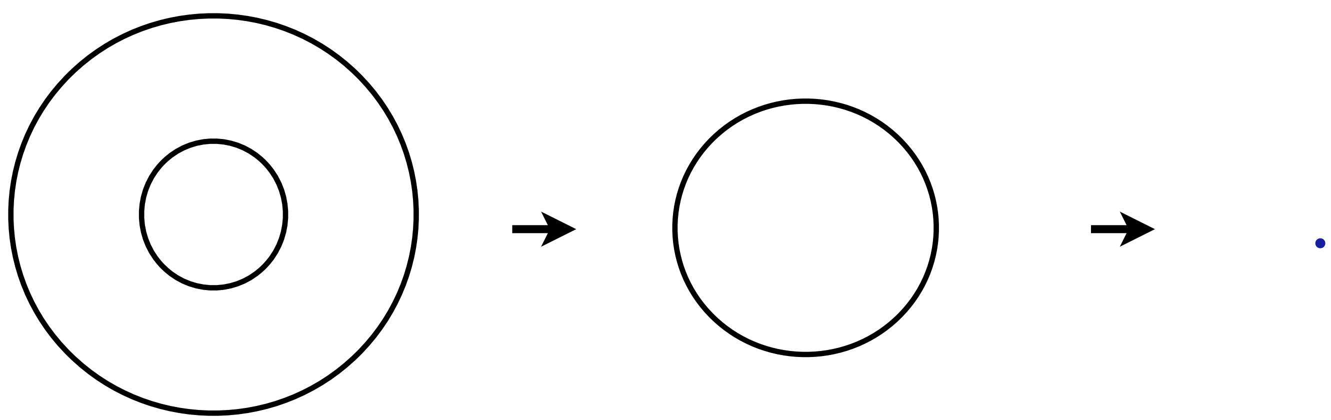
$$D(\theta) = \frac{-0.5B^{-1}\frac{d\rho}{d\theta}\int_0^\theta \rho d\theta}{1+\theta(1+\theta^2)d\ln(\rho)/d\theta}$$



Well-known solutions (mostly trivial) for curve-shortening eq.

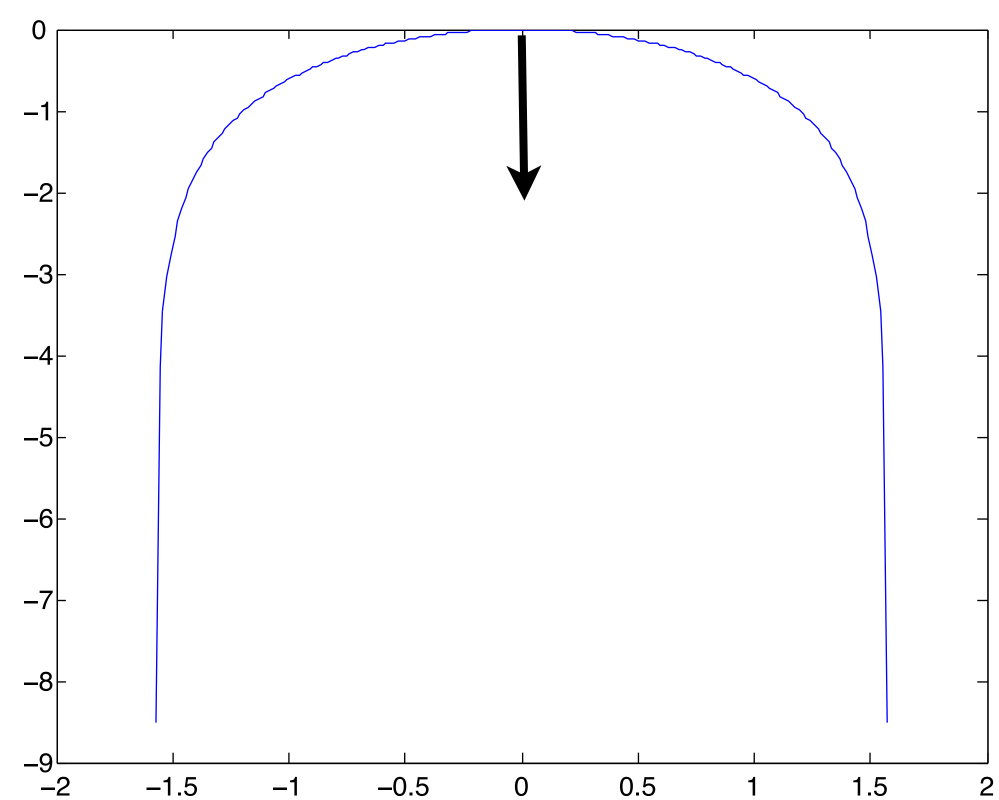
Straight lines are steady states.

Shrinking circles radius $R(t)=[2B(t_c-t)]^{1/2}$.
Tubular pipe of outer,inner radii R,r becomes simply connected at time $r^2/2B$ and disappears at time $R^2/2B$

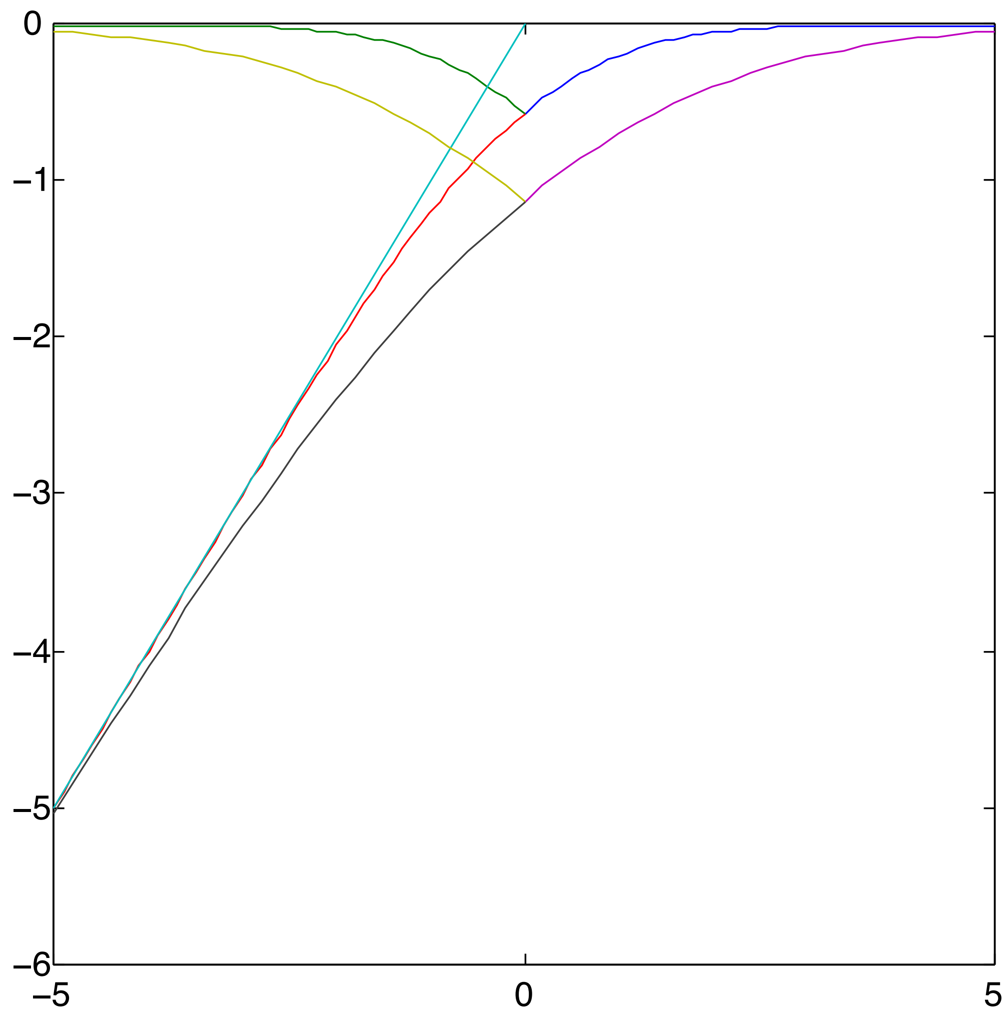


Calabi "grim reaper" travelling wave

$$y + ct = \frac{1}{c} log(cos(cx))$$



Obtuse open-angle solution = grain boundary solution.



Other similarity reductions give rotating spirals,
or Abresch-Langer 1986 “flowers”with n intersecting petals.

All of these solutions can be recovered by symmetry reductions from potential symmetries of CSL, i.e. symmetries of system

$$y_x = u \ ; \ y_t \ = \ D(u)u_x$$

$$\implies \ y_t = D(y_x)y_{xx}$$

$$\text{and} \quad u_t = \partial_x[D(u)u_x]$$

Doyle & Vassiliou 1998 classified nonlinear diffusion equations

$$u_t = \quad \partial_x[D(u)u_x]$$

according to compatibility with functional separation of variables

$$\rho(u) = f(x)g(t)$$

For $D(u)=1/(1+u^2)$, this leads to

(1) $u=y_x=\tan(x)$ -> $y=\log(\cos x) + t + \text{const}$
(vertical grim reaper),

(2) $u=x/[2(t_0-t) - x^2]^{1/2}$ -> shrinking circle

(3) $u=[e^{2(x-t)} - 1]^{-1/2}$ -> rotated (horiz) grim reaper

(4) $\dfrac{u^2+1}{u^2} \quad = \quad (1+e^{2t})\ \mathrm{cosec}^2(x),$

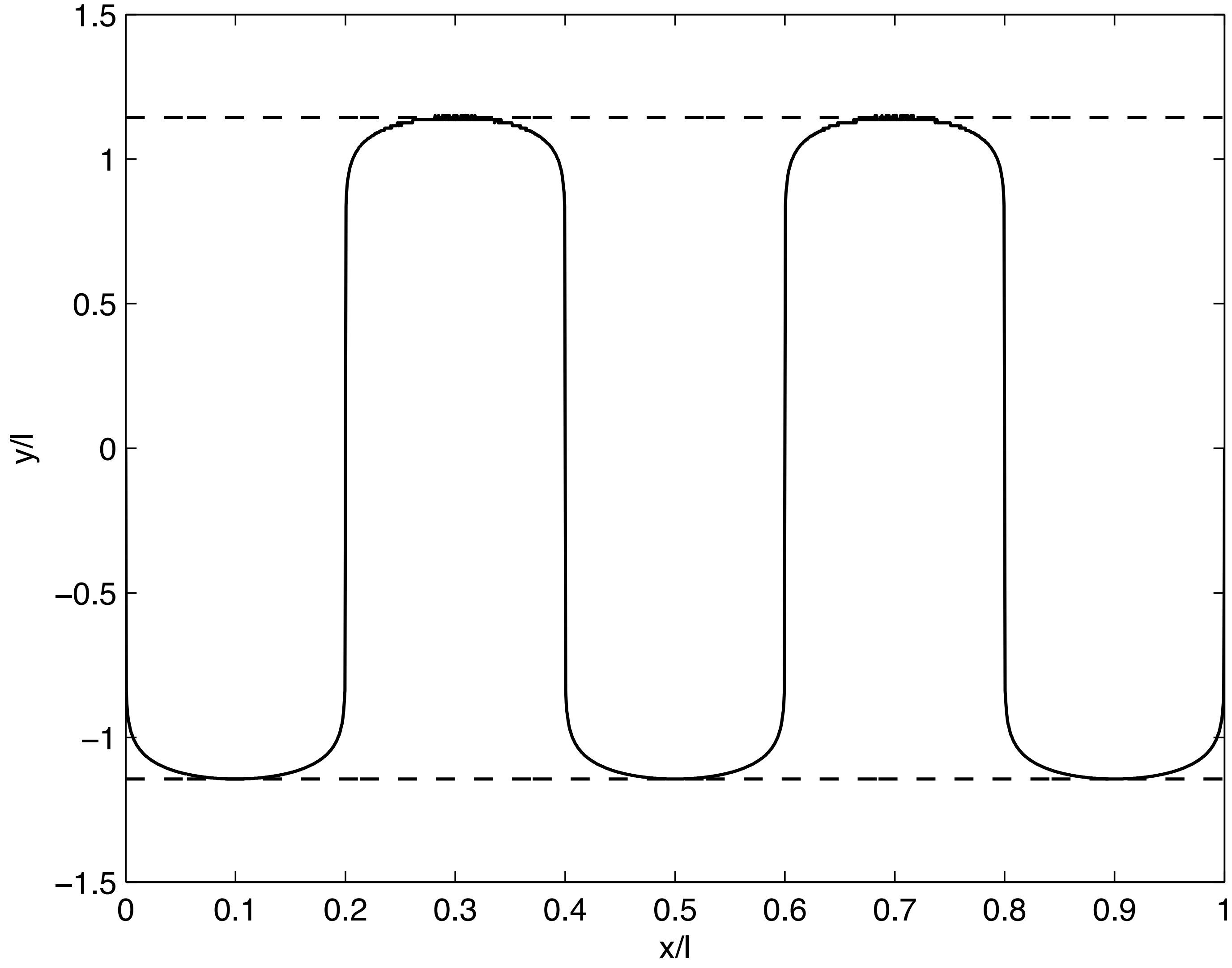
->

$$y = \frac{1}{K} log\left(\frac{\sqrt{\exp(2BK^2[t-t_0]) + cos^2(K[x-x_0])} + cos(K[x-x_0])}{\exp(BK^2[t-t_0])}\right).$$

(K, x_0, t_0 arbitrary)

- A periodic solution that can satisfy boundary conds
y=0 at x=0,L -J. R. King,

(5) $u=\cosh(x)/[e^{-2t}-\sinh^2 x]^{1/2}$ -> rotation of (4) above



$B(t-t_0)$=-0.07

---- approx bounds $y = \pm K\ [t_0 - t] + log(2)/K$

Each peak or valley is asymptotic to a grim reaper as $t \rightarrow -\infty$
Initial conds may resemble diffraction grating.

(6) $u = \pm \sin x\, [\cos^2 x - e^{2t}]^{-1/2}$

->

$$cosh(y) - e^{t_0 - t} cos(x) = 0$$

$$x^2 + y^2 = 2(t_0 - t) + O([t_0 - t]^2)$$

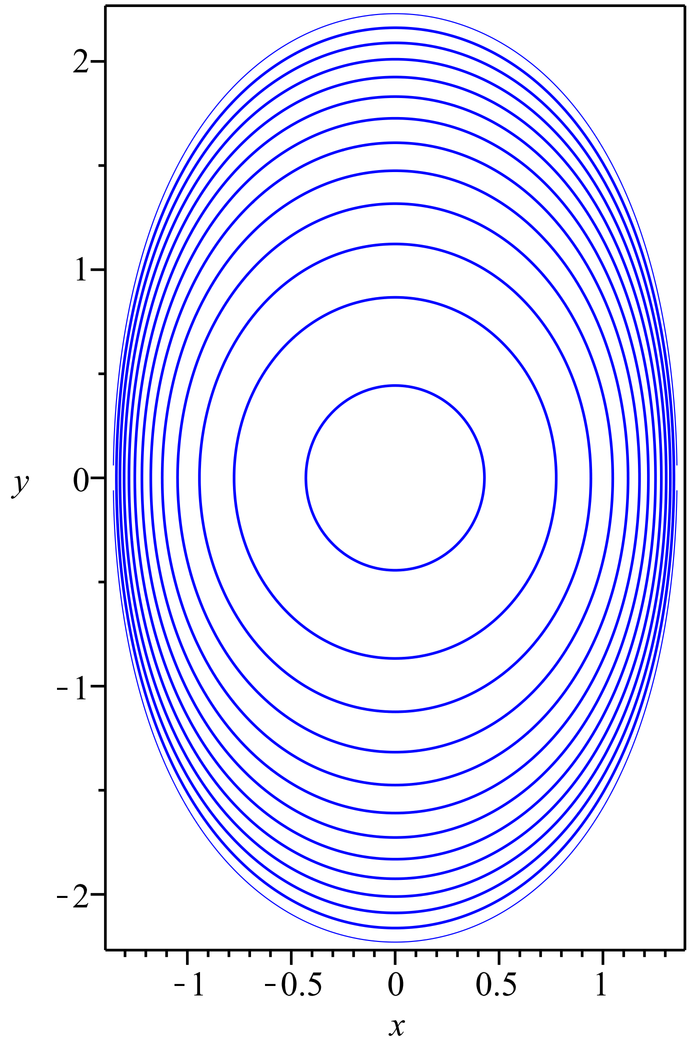
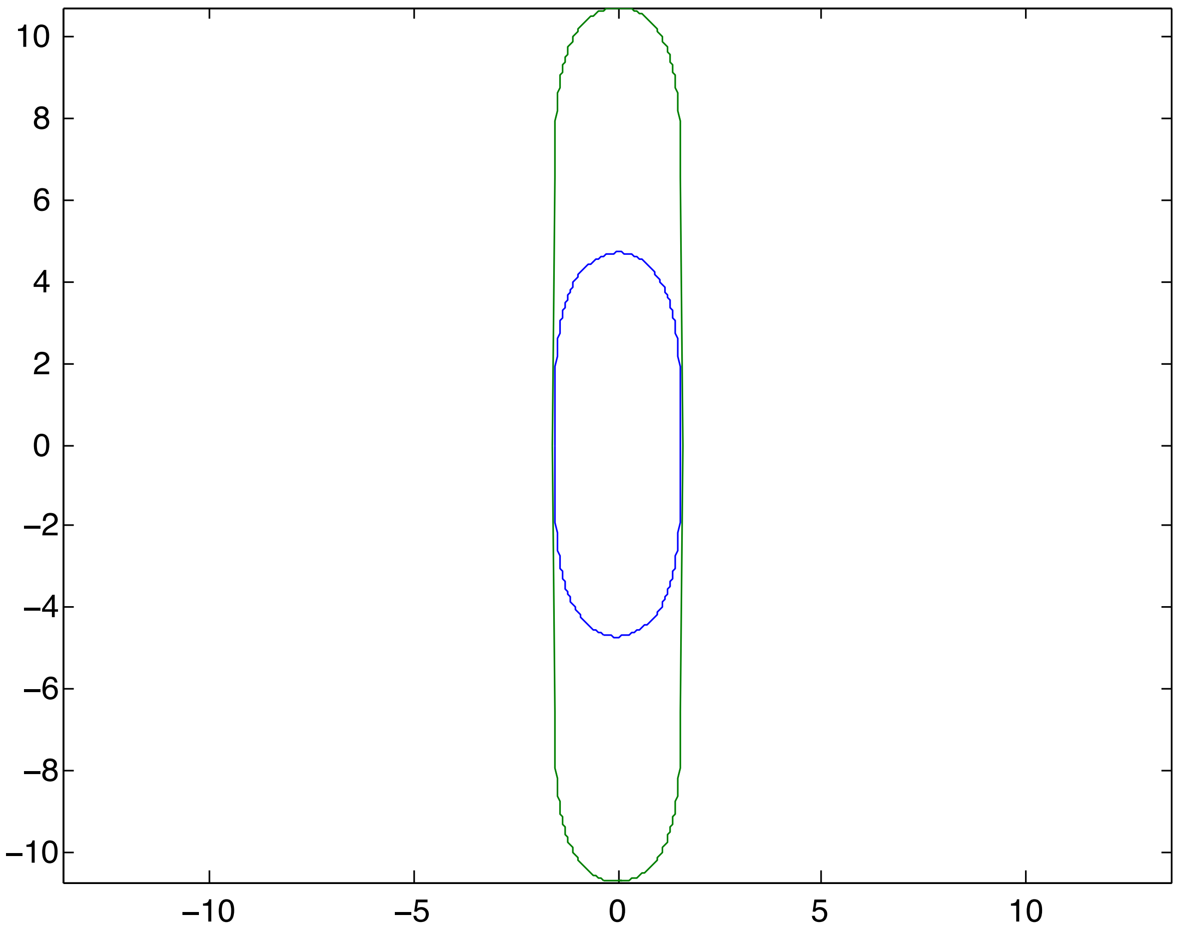


Figure 1: Evolution by heat shrinking flow of *cosh y-5cos x=0*



$t - t_0 = -10$

asymptotically approaches two coalescing grim reapers as $t \to -\infty$.

Long before extinction, $y_{max} \approx t_0 - t + log(2)$,

and near extinction, $y_{max} \approx \sqrt{2(t_0 - t)}$.

Anisotropy

$$y_t = B(y_x)\frac{y_{xx}}{1+y_x^2} = D(y_x)y_{xx}$$

Physical requirement: $0 < B_0 = D(0) < \infty$

After rotation of axes by $\pi/2$, $0 < \bar{B}_0 = \bar{D}(0) < \infty$

After rotating back,

$$D(y_x) = \frac{1}{{y_x}^2}\bar{D}\left(\frac{-1}{y_x}\right) \approx \bar{B}_0 y_x^{-2}$$

Doyle-Vassiliou classification of diffusion eqs compatible with functional separation

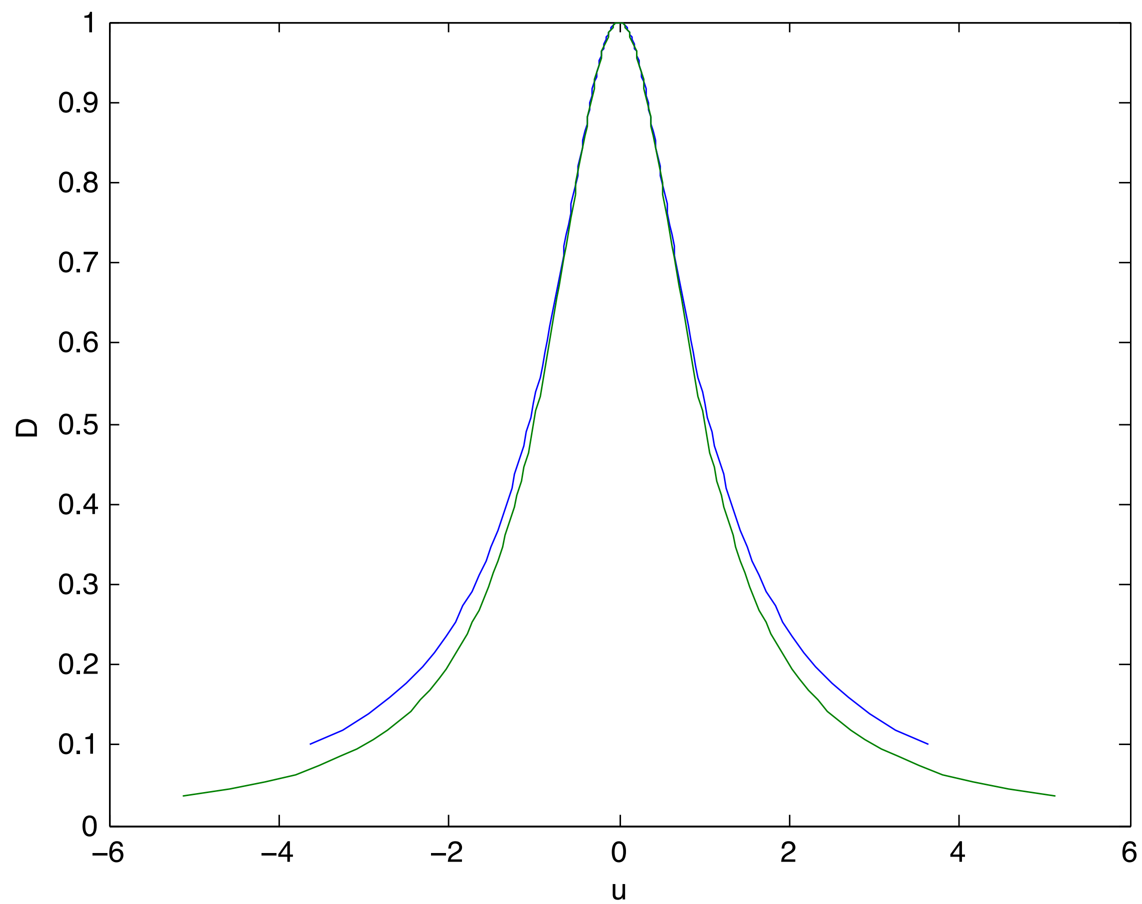
$$\log \ \rho(u) = v(x) + w(t)$$

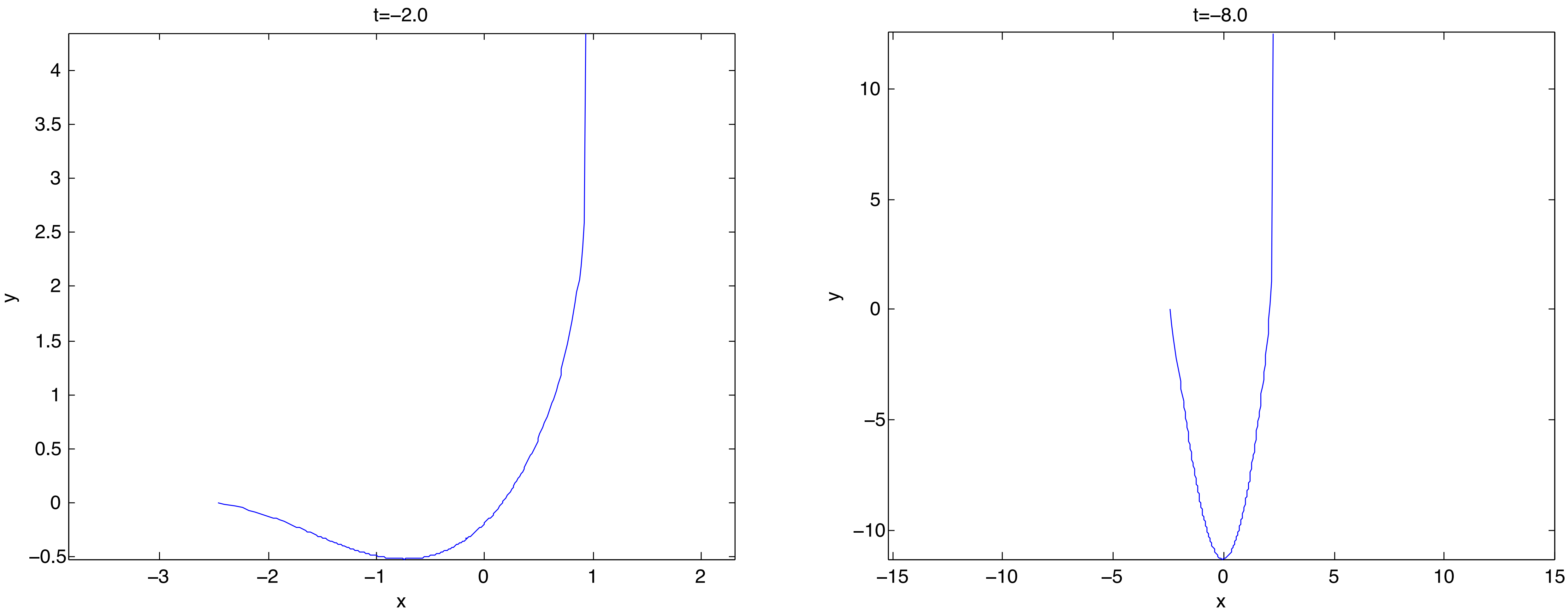
gives one more physically realistic model:

$$D(u) = D_0 cos(z(Au))$$

$$Au = \int_0^z (cos \ s)^{-3/2} ds \ ; \quad -\pi/2 < z < \pi/2$$

With A= $2^{0.5}$, $$D(u) = \frac{1}{1+u^2} \ + O(u^4) \quad \text{u small}$$
$$= (u/\sqrt{2})^{-2} \quad + O(u^{-4}) \quad \text{u large}$$


1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
D
−6
−4
−2
0
2
4
6
u



Functionally separated solution approaches grim reaper at large negative times, like others that we saw above !!

Grooving by evaporation-condensation solved exactly: PB 1989

Grooving by surface diffusion, with slope $y_x(0,t)$ constant, on nearly isotropic surface, solved by Tritscher & PB 1995.

Solved exactly when m depends on t, due to temperature dependence of surface tension-PB & Goard 2010.

For what anisotropic materials do Angenent ovals, grim reapers and diffraction grating solutions exist ?—PB & P. Vassiliou 2011

Set up reliable semi-discrete approximation
for boundary conditions that can't be treated analytically-
Zhang & Schnabel 1993, Lee 1997, PB & Goard 2012.

Integrable nonlinear discretised model with self-adapting non-uniform grid- PB, Kajiwara, Maruno & Triadis, in progress.

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