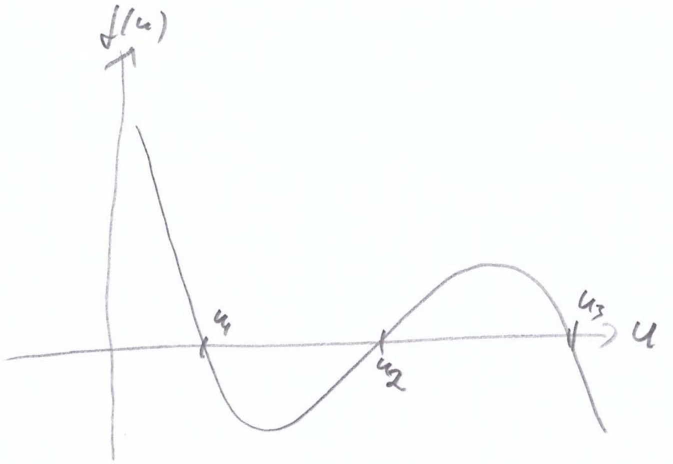
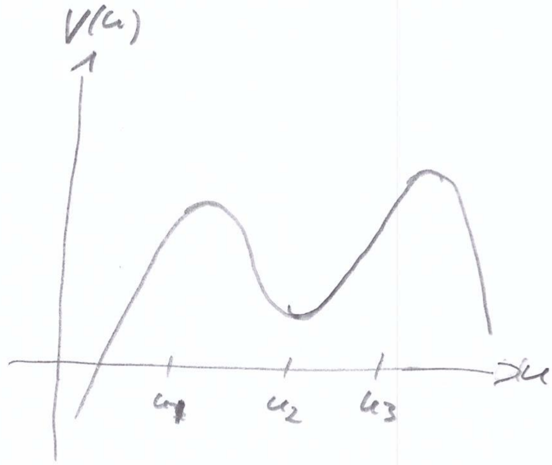
4.3 Reaktionsdiffusionssysteme

Wiederholung: Schlögl-Modell (s. Übung 5)

$$\frac{\partial}{\partial t} u(x,t) = f(u) + D \frac{\partial^2}{\partial x^2} u(x,t) \quad \text{mit } f(u) = -k(u-u_1)(u-u_2)(u-u_3)$$





mitbewegte Koordinaten: $\xi = x - ct$: $u(x,t) = u(x-ct) = u(\xi)$

$$\hookrightarrow \; -c\,u'(\xi) = f(u) + D\,u''(\xi)$$

Definiere $V(u) = \int_0^u f(\tilde{u})\, d\tilde{u} \Rightarrow \frac{\partial V}{\partial u} = f(u)$ (Potential V)

somit $D u'' = -\frac{\partial V}{\partial u} - c u'$

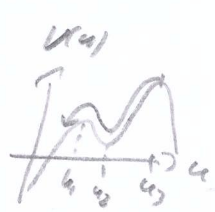
Bewegung im Potenzial $V \Rightarrow c \hat{=}$ Reibungskoeffizient!

1. Fall $c = 0$ (reibungsfrei): Energieerhaltung: $E = V(u) + \frac{1}{2} D \left(\frac{du}{d\xi}\right)^2$

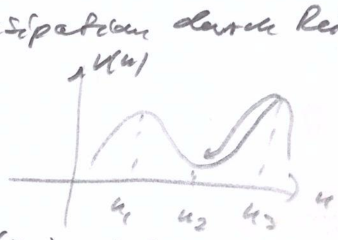
Betrachte $V(u_3) > V(u_1) \Rightarrow A := \int_{u_1}^{u_3} f(u)\, du > 0$

$\Rightarrow$ Teilchen (bei u_3 gestartet) schießt über u_1 hinaus

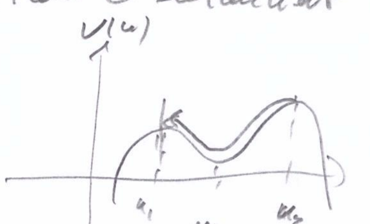
(es bleibt bei u_1 noch kinetische Energie über)



2. Fall c groß: Teilchen verliert Energie (Dissipation durch Reibung) und kommt bei u_2 zur Ruhe



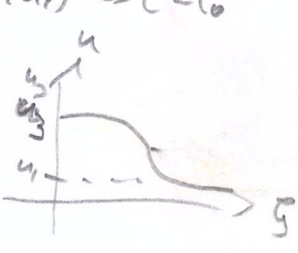
3. Fall: c balanciert Potenzialunterschied $\Delta E = V(u_3) - V(u_1) \Rightarrow c = c_0$



$\Rightarrow$ Teilchen erreicht gerade so u_1

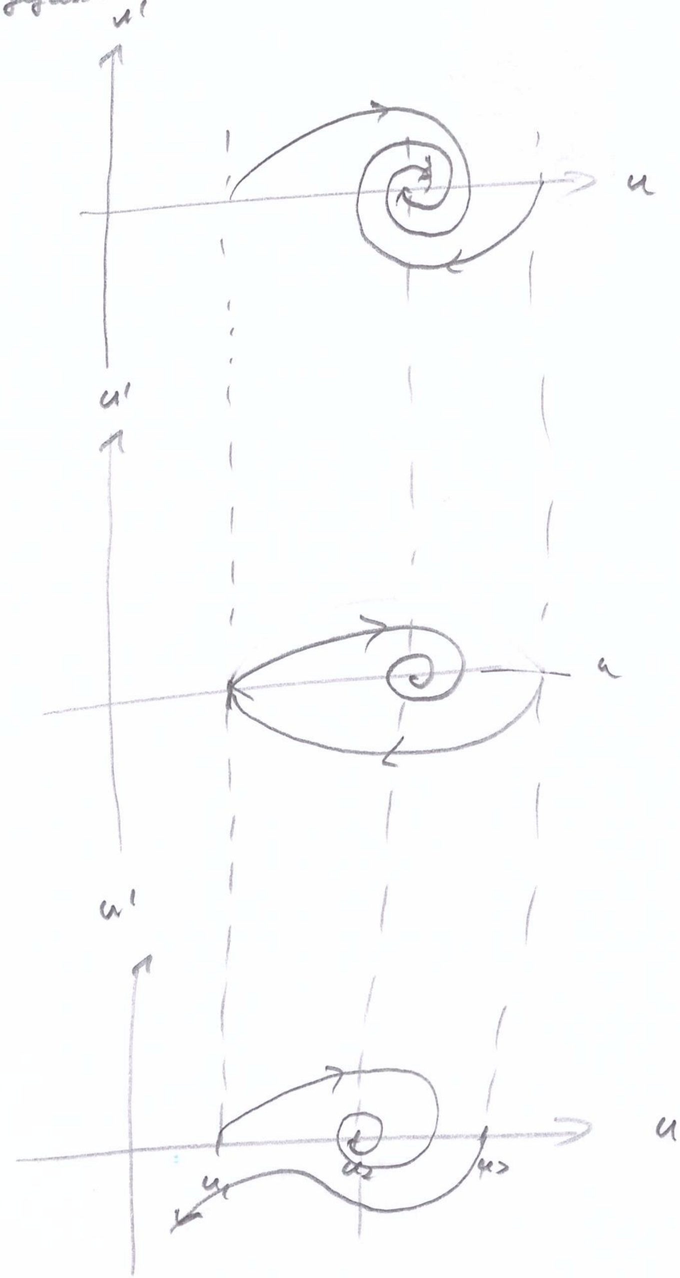
$\Rightarrow$ Lösung: $u \to u_3$ für $\xi \to -\infty$

$u \to u_1$ für $\xi \to +\infty$



(Übergangswellen) fronten (T

Zusammengefasst:



$C > C_0$

$A < 0$

$C = C_0$

$A = 0$

$C < C_0$

$A > 0$

$$A = \int_{u_1}^{u_3} -k\,(u-u_1)(u-u_2)(u-u_3)\,du = 0$$

equal-area rule

Ursprung: autokatalytische Reaktionen:

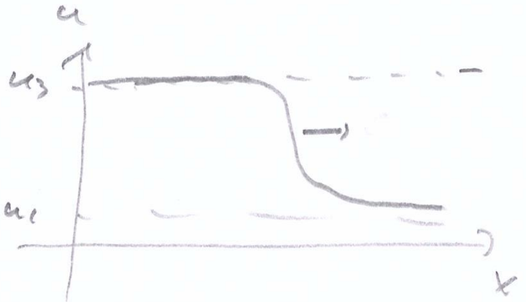
$$M + 2X \underset{k_2}{\overset{k_1}{\rightleftharpoons}} 3X \quad , \quad X \underset{k_4}{\overset{k_3}{\rightleftharpoons}} N$$

Reaktionskinetik: $\dot{X} = k_1 M X^2 - k_2 X^3 - k_3 X + k_4 N$

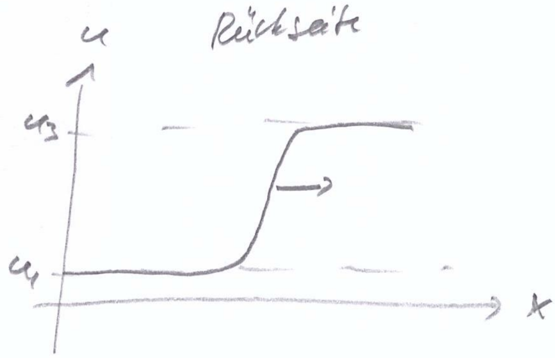
mit M und N konstant, folgt das Schlögl-Modell

wandernde Pulse (travelling pulses)

Vorderseite



Rückseite



$$\frac{\partial u}{\partial t} = f(u,v) + D\,\frac{\partial^2 u}{\partial x^2} \Rightarrow A(v) = \int_{u_1}^{u_3} f(u,v)\,du$$

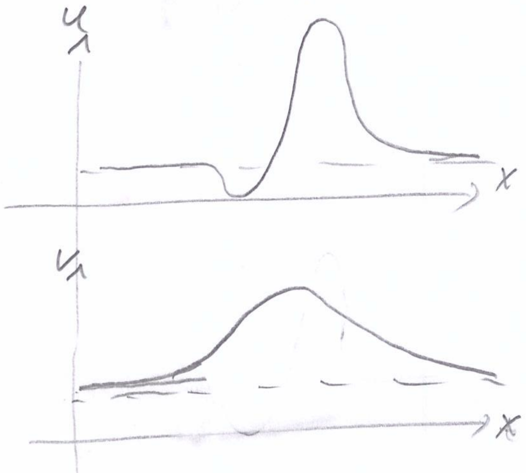
$A > 0$: Anregung (Ignition)

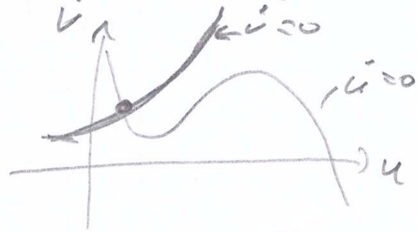
$A < 0$: Auslöschung (Quenching)

u : Aktivator , v : Inhibitor

$\Rightarrow$ 2. Variable v fängt Dynamik ein: $\frac{\partial v}{\partial t} = -\frac{1}{\tau}\left(v - \bar{v}(u)\right)$

Gleichgewichtszustand (ggf. u-Abhängig)





Bsp: FitzHugh-Nagumo-Modell (s. Blatt 5)

$$\varepsilon \frac{\partial u}{\partial t} = u - \frac{u^3}{3} - v + D\,\frac{\partial^2 u}{\partial x^2}$$

$$\frac{\partial v}{\partial t} = u + a$$

Brüsselator-Modell

$$A \to X \;,\; B + X \to Y + D \;,\; 2X + Y \to 3X \;,\; X \to E$$

$\Rightarrow$ u: Konzentration von X, V: Konzentration von Y:

$$\frac{\partial u}{\partial t} = A - Bu + u^2 v - u + D_u \frac{\partial^2 u}{\partial x^2}$$

$$\frac{\partial v}{\partial t} = Bu - u^2 v + D_v \frac{\partial^2 v}{\partial x^2}$$

$\Rightarrow$ Turing-Muster

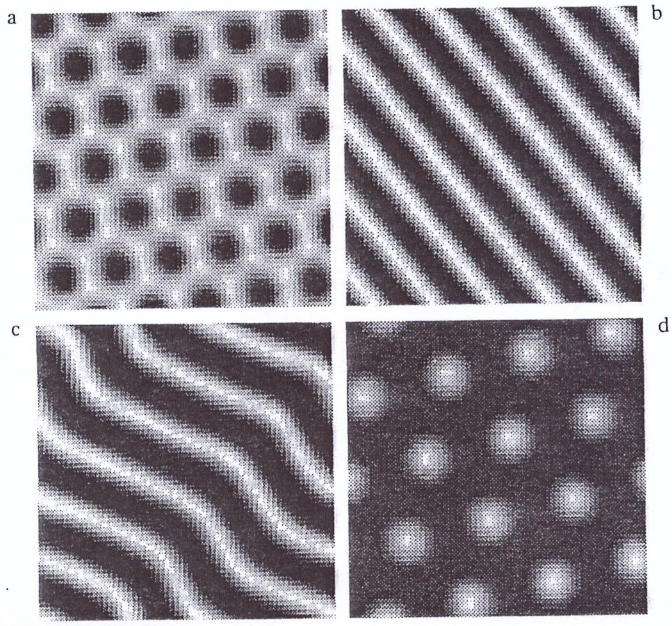


Fig. 5.15a–d. Basic types of two-dimensional Turing-patterns obtained by the numerical simulation of the Brusselator model: (**a**) a hexagonal lattice of cells, (**b**) stripes, (**c**) zig-zag stripes, and (**d**) a hexagonal lattice of spots. (From [5.32])

aus P. Borckmann, A. DeWitt, G. Dewel, Physica A 188, 171 (1992)

Competition in ramped Turing structures

Belousov-Zhabotinskii-Reaktion (BZ-Reaktion)

beschreibbar durch 2 effektive Komponenten:

$$\frac{\partial u}{\partial t} = u(1-u) - \frac{v(u-a)}{u+a} + D_u \frac{\partial^2 u}{\partial x^2} \qquad , a,b>0$$

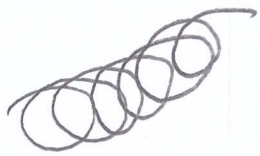
$$\frac{\partial v}{\partial t} = -\frac{1}{\tau}(v-bu) + D_v \frac{\partial^2 v}{\partial x^2} \qquad \tau \gg 1$$

(v: langsam)

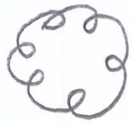
Spiralwellen möglich: stationär oder wandernd

Spiral tip auf Kreis

Spiraltip auf Kurve



oder



Muster in 3D: Scroll waves

Scroll rings

twisted scrolls

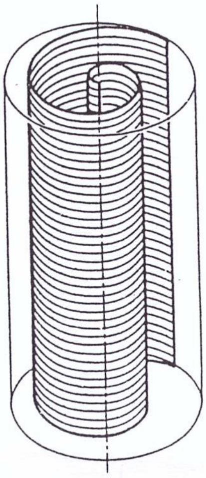


Fig. 3.31. Straight scroll vortex

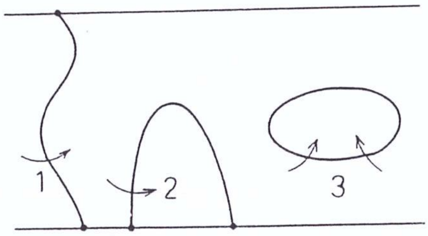


Fig. 3.32. Possible deformations of the vortex filament. Arrows indicate the direction of rotation

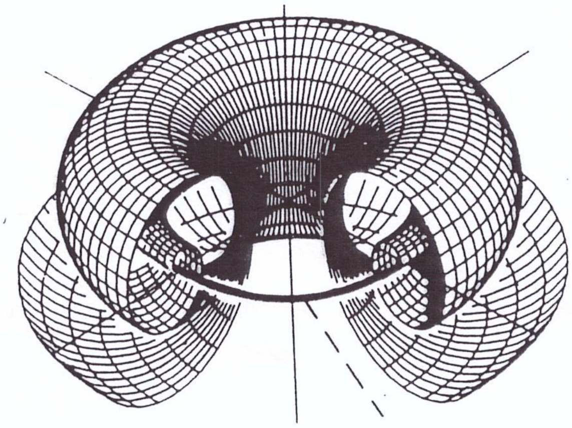


Fig. 3.33. Scroll ring

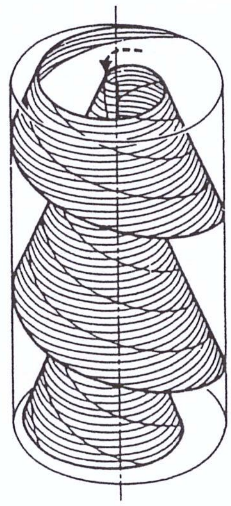


Fig. 3.34. Straight twisted scroll