INTERNATIONAL ATOMIC ENERGY AGENCY
UNITED NATIONS EDUCATIONAL, SCIENTIFIC AND CULTURAL ORGANIZATION

INTERNATIONAL CENTRE FOR THEORETICAL PHYSICS
34100 TRIESTE (ITALY) - P.O.B. 586 - MIRAMARE - STRADA COSTIERA 11 - TELEPHONE: 2240-1
CABLE: CENTRATOM - TELEX 460392 - I

SMR/390 - 7

WORKING PARTY ON "FRACTURE PHYSICS"
(29 May - 16 June 1989)

FROM DISLOCATION DYNAMICS TO SELF ORGANIZATION OF DISLOCATIONS
(Background Material)

G. ANANTHAKRISHNA
Indira Gandhi Centre for Atomic Research
Materials Science Laboratory
603 102 Kalpakkam
India

PROCESSES

Random variable ξ has many realizations, say ξ_i, $i = 1$ to N, then, it is characterized by $\langle \xi \rangle, \langle \xi^2 \rangle, \cdots \langle f(\xi) \rangle$

$$\langle \xi \rangle = \lim_{n \to \infty} \left(\sum_{i=1}^{n} \xi_i \right) / n$$

Define $\Theta(z) = \begin{cases} 1 & z > 0 \\ 0 & z < 0 \end{cases}$

Probability of $\xi < x$, distribution function, $P(\xi < x) = \langle \Theta(x - \xi) \rangle$

$$= \lim_{n \to \infty} \left(\sum_{i=1}^{n} \epsilon_i \right) / n \quad , \quad \epsilon = \Theta(x - \xi)$$

$$W_\xi(x) = \frac{dP}{dx} = \langle \delta(x - \xi) \rangle$$

$$\int W_\xi(x)\, dx = 1$$

For simplicity drop subscript ξ which simply refers to the random variable ξ.

Characteristic function

$$f_\xi(u) = \langle e^{iu\xi} \rangle = \int e^{iu\xi} W(\xi)\, d\xi$$

$$W(\xi) = \frac{1}{2\pi} \int e^{-iu\xi} f(u)\, du$$

$$f(u) = \left\langle \sum \frac{(iu)^n}{n!} \xi^n \right\rangle = \sum \frac{(iu)^n}{n!} m_n$$

m_n = moments of $\xi = \langle \xi^n \rangle$

$f(0) = 1$; expansion of $f(u)$ around $u = 0$

$$f(u) = \exp \sum \frac{(iu)^n}{n!} k_n$$

Expansion of $\ln f(u)$ around $u = 0$

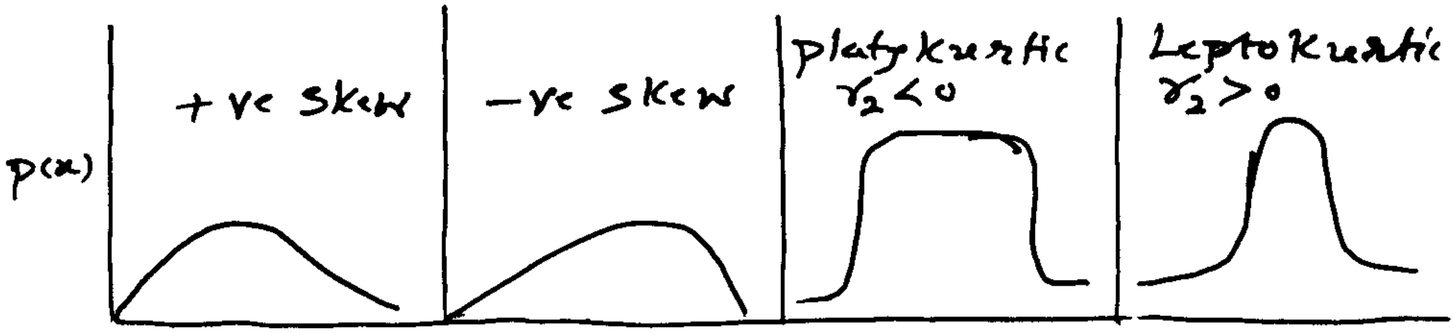
k_n = cumulants

$k_1 = m_1$; $k_2 = m_2 - m_1^2$; $k_3 = m_3 - 3m_1m_2 - 2m_1^3$

$k_4 = m_4 - 3m_2^2 - 4m_1m_3 + 12m_1^2m_2 - 6m_1^4$

k_2 = variance , γ_s = coef. of asym $= \dfrac{k_3}{k_2^{3/2}}$

γ_k = coef. of excess $= k_4 / k_2^2$



Joint probability :

$$W_{\xi_1,\dots\xi_n}(x_1,\dots x_n) = \langle \delta(\xi_1 - x_1)\cdots\delta(\xi_n - x_n)\rangle$$

Drop subscript

$$W(\xi_1 \cdots \xi_k) = \int W(\xi_1,\dots,\xi_k,\xi_{k+1},\dots\xi_n)\, d\xi_{k+1}\cdots d\xi_n$$

$$\langle f(\xi_1\cdots\xi_n)\rangle = \int f(\xi_1\cdots\xi_n)\, W(\xi_1\cdots\xi_n)\, d\xi_1\cdots d\xi_n$$

Conditional probability :

$$P(\xi_1 | \xi_2) = W(\xi_1, \xi_2)/W(\xi_1)$$

$$P(\xi_1\cdots\xi_k | \xi_{k+1},\cdots\xi_n) = \frac{W(\xi_1\cdots\xi_n)}{W(\xi_1\cdots\xi_k)}$$

Gaussian

$$W(\xi_1 \cdots \xi_n) = (2\pi)^{-n/2} \| \det k_2(t_\alpha; t_\beta) \|^{1/2}$$
$$\times \exp -\tfrac{1}{2} \sum a_{\alpha\beta} [\xi_\alpha - k_2(t_\alpha)] [\xi_\beta - k_2(t_\beta)]$$

$$a_{\alpha\beta} = [k_2(t_\alpha, t_\beta)]^{-1}$$

$$k_2 = \begin{bmatrix} k_{11} & \cdots & k_{1n} \\ \vdots & \ddots & \vdots \\ k_{n1} & \cdots & k_{nn} \end{bmatrix}$$

$$W(\xi_1 \xi_2) = \frac{\exp\left[- \dfrac{\xi_1^2 - 2R_2 \xi_1 \xi_2 + \xi_2^2}{2\sigma^2(1-R_2^2)} \right]}{2\pi\sigma^2 (1-R_2^2)^{1/2}}$$

$$R_2(\xi_1, \xi_2) = \frac{k_2(\xi_1, \xi_2)}{\sigma(\xi_1)\sigma(\xi_2)} = \text{correl}^n \text{ coef.}$$

Spectral density: $\xi = \xi_t = \xi(t)$

$$S[\xi, \omega] = 2 \int_{-\infty}^{\infty} e^{i\omega t} \langle \xi_0 \xi_t \rangle \, dt$$

$$\langle \xi_0 \xi_t \rangle = k(t) + m_1^2$$

Cross spectral density

$$S[\xi, \eta; \omega] = 2 \int_{-\infty}^{\infty} e^{i\omega t} \langle \xi_0 \eta_t^* \rangle \, dt$$

Stationary: statistical properties are time invariant, i.e. all W's

$$W_n(y_1 t_1; y_2 t_2; \cdots y_n t_n) = W_n(y_1; t_1 + t; \cdots ; y_n\, t_n + t)$$

Purely Random

$$W_2(y_1 t_1 ; y_2 t_2) = W_1(y_1 t_1) W_1(y_2 t_2)$$

Markoff process: Depends on just the previous state

$$W_{n+1}(y_1 t_1 ; \cdots ; y_n t_n \mid y_{n+1} t_{n+1}) = W_2(y_n t_n \mid y_{n+1} t_{n+1})$$

Ex: $\int W_3(y_1 y_2 y_3)\, dy_2 = W_2(y_1 y_3) = W(y_1) P(y_3 | y_1)$

$$= \int W_2(y_1 y_2)\, P(y_3 | y_2 y_1)\, dy_2$$

$$= \int P(y_1 | y_2) W(y_1) P(y_3 | y_2)\, dy_2$$

$$\boxed{P(y_1 | y_3) = \int P(y_1 | y_2) P(y_2 | y_3)\, dy_2}$$

Smoluchowski's eqn.

Fokker Planck Eqn

$$P(x | y ; t + \Delta t) = \int P(x | z ; t) P(z | y ; \Delta t)\, dz$$

use $R(y)$, arbitrary diff. function

$$\frac{1}{\Delta t}\int [P(x | y ; t + \Delta t) - P(x | y, t)] R(y)\, dy$$

expand $R(y)$ around $R(z)$:

$$\int (y - z)^n dy\, P(z | y, \Delta t) = a_n(z, \Delta t)$$

From this we get

$$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial y} a_1 P + \frac{1}{2}\frac{\partial^2}{\partial y^2} a_2(y) P(y)$$

n variable F·P Eqn

$$\frac{\partial P(y_1 \cdots y_n)}{\partial t} = -\sum_i \frac{\partial}{\partial y} A_i(y)\, P(y) + \frac{1}{2} \sum_i \frac{\partial^2}{\partial y_i\, \partial y_j} B_{ij}(\vec{y})\, P(y)$$

Connection between F.P. Eqn and Langevin Eqn:

$$\dot{x} = c(x) + \beta(x)\, \eta(t)$$

$$\langle \eta(t) \rangle = 0 \ ; \ \langle \eta(t)\, \eta(t') \rangle = 2\epsilon\, \delta(t-t')$$

F.P. Eqn $$\frac{\partial P}{\partial t} = -\frac{\partial}{\partial x}\left[c(x) + \epsilon\, \beta(x)\, \beta'(x)\right] P(x) + \epsilon \frac{\partial^2}{\partial x^2} \beta^2(x)\, P(x)$$

Master Eqn

$$\frac{dP_n}{dt} = \sum_{n'} \left(W_{nn'} P_{n'} - W_{n'n} P_n \right)$$

Detailed balance

$$W_{nn'} P_{n'}^{eq} = W_{n'n} P_n^{eq}$$

$\Longrightarrow$ $t \to \infty$ eqm is attained.

ELEMENTS (SUMMARY) OF NONLINEAR METHODS

Consider a system with x_i, $i = 1$ to n

dynamical variables

$$\frac{dx_i}{dt} = F_i(\{x_j\};\{\lambda_k\}) \qquad \begin{matrix} i,j = 1 \text{ to } n \\ k = 1 \text{ to } m \end{matrix}$$

λ_k drive parameters

For systems where spatial dependence enters, we may have ∇_j also

$$\frac{dx_i}{dt} = F_i(\{x_j\}, \nabla_j; \{\lambda_k\})$$

First find homogeneous steady state by setting $\dot{x}_i = 0$ and obtain x_i^0. Then perform linear stability analysis by linearizing F_i around x_i^0, i.e. $x_i^0 + z_i = x_i$

$$\frac{\delta z_i}{dt} = \sum_j \left.\frac{\partial F_i}{\partial x_j}\right|_{x_j = x_j^0} \delta z_i$$

Solution is $\vec{z} = (\exp \underline{\underline{A}}\, t)\, \vec{z}(t_0)$

case 1: ω_i's are real

some $\omega_j < 0 \longrightarrow \omega_j > 0$

[illegible] SPATIAL PATTERN

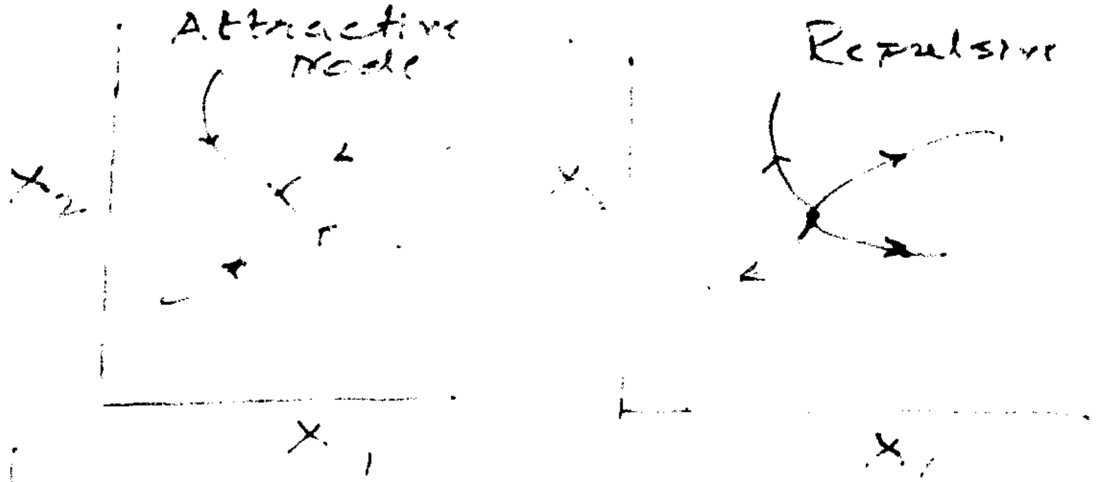
Case 2: ω_i complex, $Re\,\omega < 0 \xrightarrow{\lambda} Re\,\omega > 0$

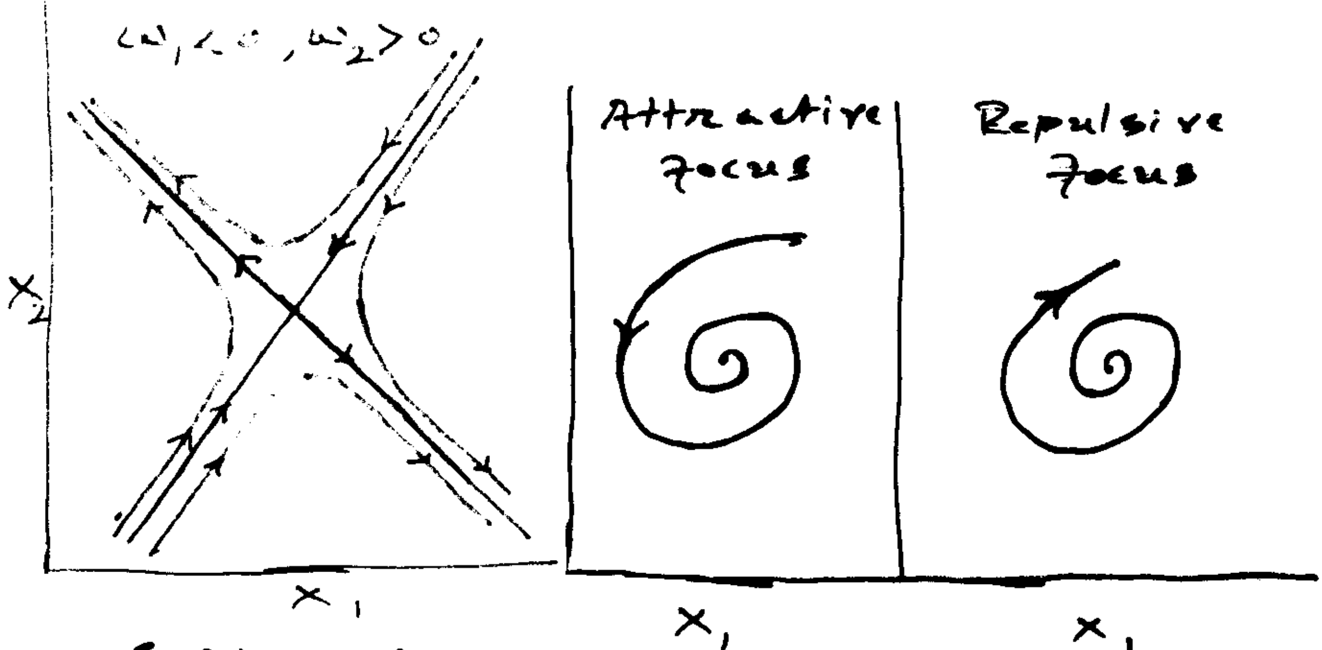
Temporal oscillations

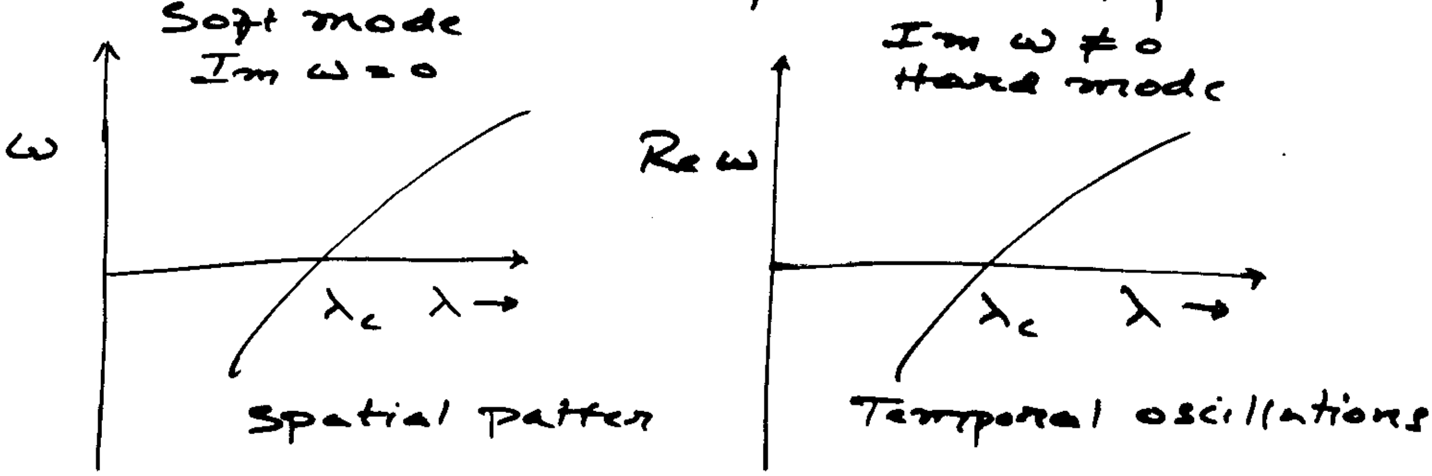
or

HARD MODE

$\underline{i = 2}$, MODE, $\omega_i < 0;\ i = 1, 2$ or $\omega_i > 0$

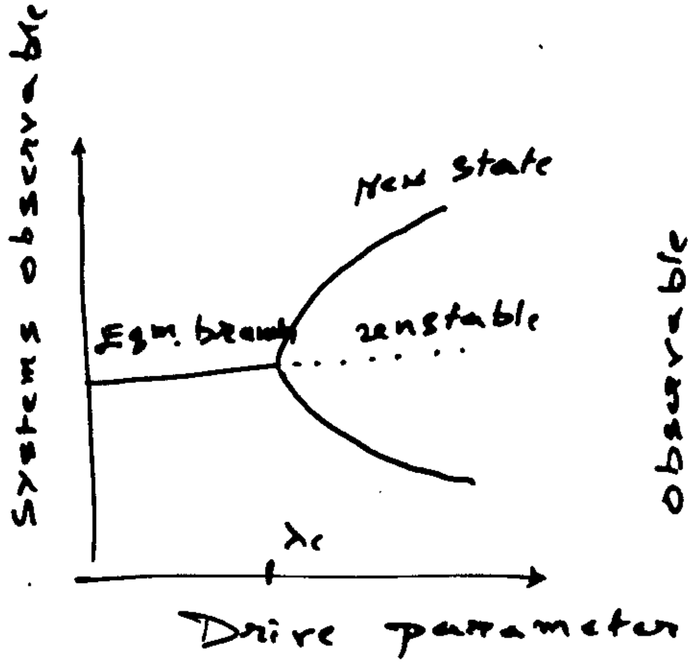


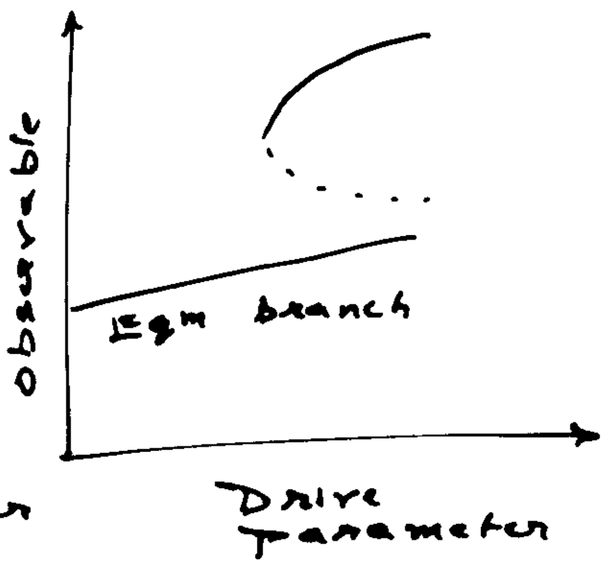




Bifurcation:

Qualitative change in the nature of solution occurs as the drive paramet is varied across a critical value.



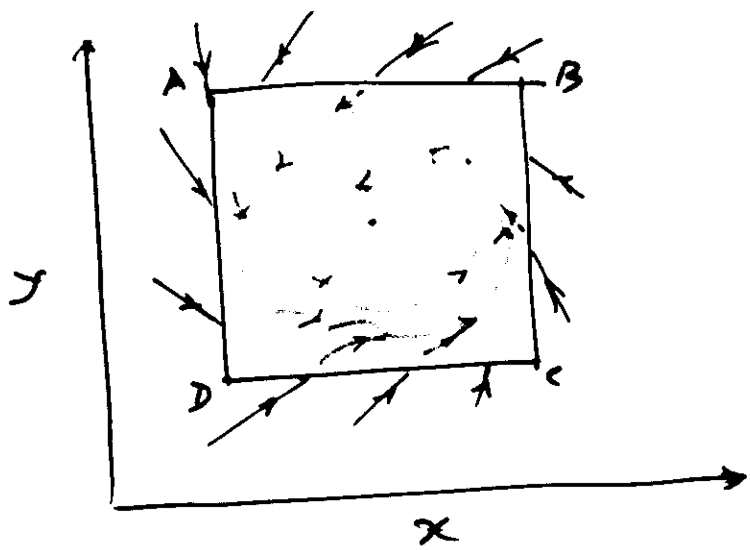


Smooth transition since the new brach emerges from the equillibrium brach

Abrupt transition

If we obtain unstable focus as the drive parameter is varied (during linear stability analysis, it implies that the trajectory is locally unstable with a growing oscillatory behaviour. However

The global stability controlled by only the nonlinear terms, stabilize this growth. This give rise to limit cycle oscillations. Limit cycle solutions are periodic solutions (i.e, one dimensional attractor)



There is surface ABCD enclosing the focus into which all the trajectories are attracted. From the repulsive focus they move outwards. So they (trajectories) have an attractor. In the simplest case they are the limit cycles.

~~[illegible]~~ Near λ_c some modes are fast compared the slow modes (remember $Re\,\omega \to 0$ for some modes with $Im\,\omega \neq 0$). They can be eliminated. This is called adiabatic elimination of modes. In this case the slow modes determine the new structure or phase and the principle is called slaving principle in self organization.