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Numerical Methods for Differential Equations in Physics

Time stepping: $$\partial_t U = LU + N(U)$$

Steady state solving: $$0 = LU + N(U)$$

Linear Stability Analysis: $$\lambda u = Lu + N_U u$$

Navier-Stokes Equations

$$\begin{aligned}
\partial_t U &= -(U \cdot \nabla)U - \nabla P + \nu \Delta U \\
&= -(I - \nabla\nabla^{-2}\nabla\cdot)(U \cdot \nabla)U + \nu \Delta U \\
&= N(U) + L\,U
\end{aligned}$$

$$\begin{aligned}
N_U u &\equiv -(U \cdot \nabla)u - (u \cdot \nabla)U \\
A_U u &= N_U u + Lu
\end{aligned}$$

Must solve

$$\lambda u = Lu + N_U u$$

Linear Stability Analysis

$$\lambda u = Lu + N_U u$$

How to calculate eigenpairs (λ, u)?

1) Direct: Diagonalisation = QR decomposition

Storage: M^2 **Time: M^3**

3D case with $M_x = M_y = M_z = 10^2 \implies M = 10^6$

$M^2 = 10^{12}$ $M^3 = 10^{18}$

2) Iterative: Calculate a few desired eigenpairs.

Use only matrix-vector products $u \to Au$

To diagonalise an arbitrary matrix,

$$\left.\begin{array}{l}\textbf{Each product } u \to Au \textbf{ requires } M^2 \textbf{ operations}\\ \textbf{Generating } M \textbf{ eigenpairs requires } M \textbf{ iterations}\end{array}\right\} M^3$$

Can gain:

If A **is structured or sparse, then** $u \to Au$ **takes** $\sim M$ **ops**

Aim method at desired eigenvalues.

Power method

$$A\psi_j = \lambda_j \psi_j \qquad \text{where } |\lambda_1| > |\lambda_2| > \cdots$$

$$u = \sum_j u_j \psi_j$$
$$Au = \sum_j u_j \lambda_j \psi_j$$
$$\vdots$$
$$A^N u = \sum_j u_j \lambda_j^N \psi_j = \lambda_1^N u_1 \left(\psi_1 + \psi_2 \frac{u_2}{u_1} \left(\frac{\lambda_2}{\lambda_1} \right)^N + \psi_3 \frac{u_3}{u_1} \left(\frac{\lambda_3}{\lambda_1} \right)^N + \ldots \right)$$

$\uparrow$ converges to first evec $\uparrow$ first error term

Rayleigh quotient:

$$\frac{\langle A^{N-1}u, A^N u\rangle}{\langle A^{N-1}u, A^{N-1}u\rangle} \approx \frac{\langle \lambda_1^{N-1} u_1 \psi_1, \lambda_1^N u_1 \psi_1\rangle}{\langle \lambda_1^{N-1} u_1 \psi_1, \lambda_1^{N-1} u_1 \psi_1\rangle} = \lambda_1$$

What if we want more than one eigenvalue?

What if we want an eigenvalue which is not the dominant one (largest $|\lambda|$)?

Leading Eigenvalues: $A\Psi = \lambda\Psi$

$$u \to Au \to A^2u \to A^3u \to A^4u \to A^5u \to A^6u \to A^7u$$

Power Method

$$A^2u \to v = \frac{A^n u}{\|A^n u\|}$$

$$\lambda \approx \langle v, Av \rangle \qquad \Psi \approx v$$

Arnoldi Decomposition

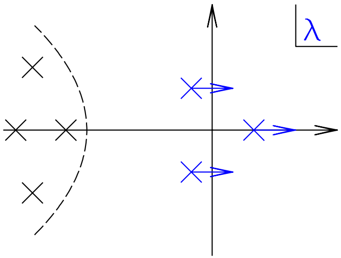
$$\{A^4u, \dots, A^7u\} \to \begin{bmatrix} v_1 & v_2 & \cdots & v_K \\ \downarrow & \downarrow & \downarrow & \downarrow \\ \downarrow & \downarrow & \downarrow & \downarrow \end{bmatrix}$$

$$\underset{K\times K}{H} = \underset{K\times N}{V^T}\,\underset{N\times N}{A}\,\underset{N\times K}{V} \qquad H_{ij} \equiv \langle v_i, Av_j \rangle$$

$$\underset{N\times N}{A} \approx \underset{N\times K}{V}\,\underset{K\times K}{H}\,\underset{K\times N}{V^T} \qquad AV \approx VH$$

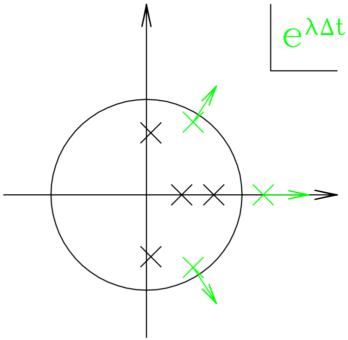
$$H\phi = \lambda\phi \qquad AV\phi \approx VH\phi$$
$$= \lambda V\phi$$

Matrix Transformations

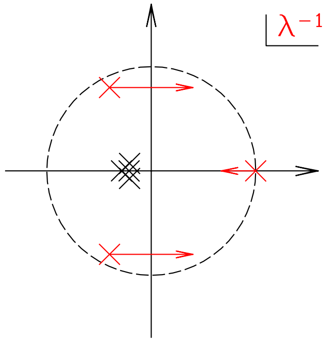


If $\boldsymbol{A\,u = \lambda\,u}$

then $\boldsymbol{f(A)\,u = f(\lambda)\,u}$



$\boldsymbol{f(A) = e^{A\Delta t}}$



$\boldsymbol{f(A) = A^{-1}}$

$\boldsymbol{f(A) = \sum_j f_j A^j}$

$\boldsymbol{f_j}$ **chosen dynamically to extract desired eigenvalues: principle of** ARPACK **(Sorensen et al.)**

Exponential Power Method

$$u_{n+1} = (I - \Delta t L)^{-1}(I + \Delta t N_U) u_n \approx e^{\Delta t (L + N_U)} u_n$$

Approximation valid for $\Delta t \ll 1$

Time-stepping linearized evolution equation

Enhancement factor at each iteration is

$$\left| \frac{e^{\Delta t \lambda_1}}{e^{\Delta t \lambda_2}} \right| \gtrsim 1 \qquad \text{where } \lambda_1 > \lambda_2 > \cdots$$

Inverse Power Method

$$u_{n+1} = (L + N_U)^{-1} u_n$$

Solve matrix equation using iterative method if necessary

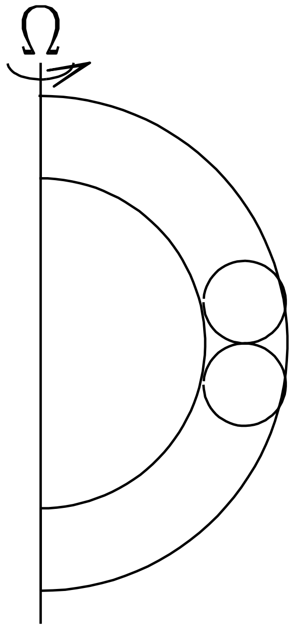
Enhancement factor at each iteration is

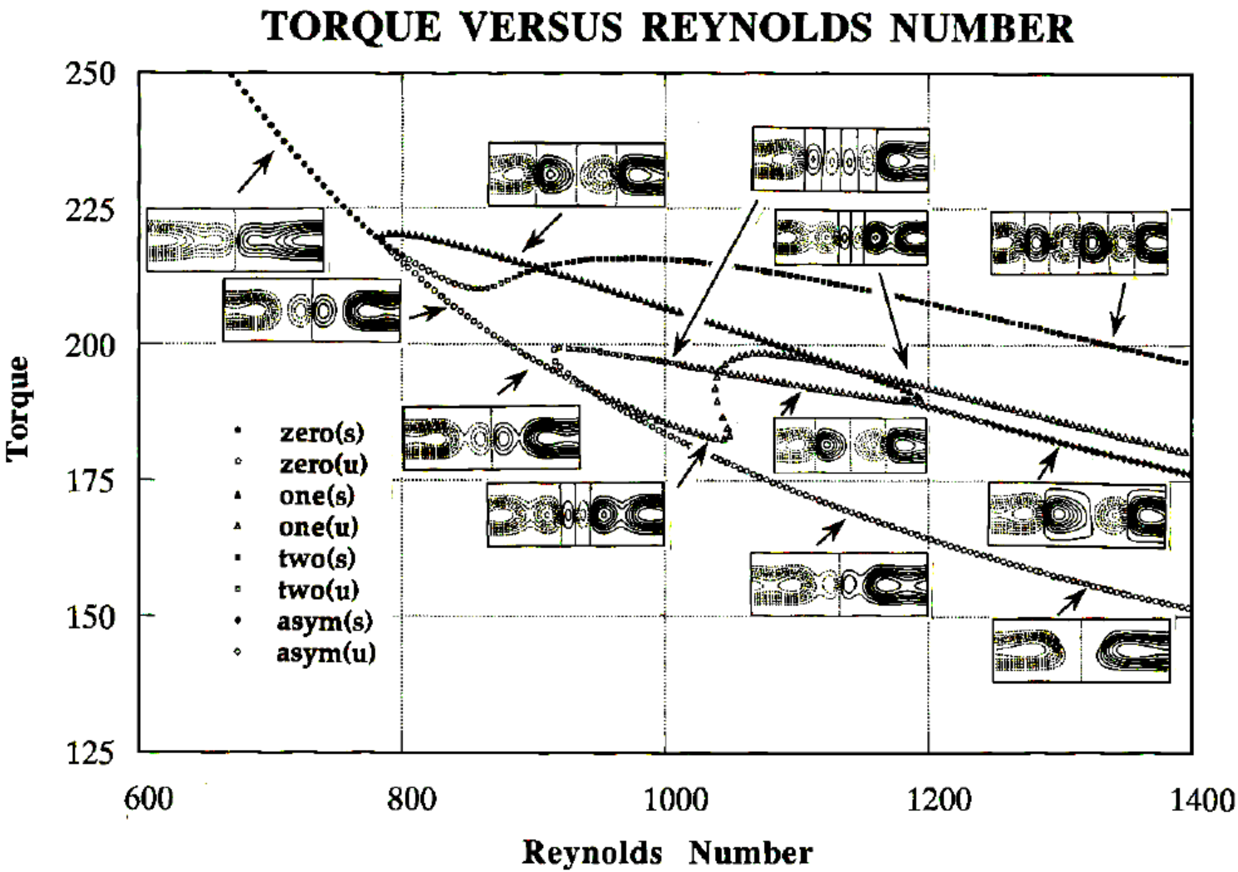
$$\left|\frac{\lambda_2}{\lambda_1}\right| \gg 1 \text{ for } \lambda_1 \approx 0$$

Can shift to find eigenvalues closest to s

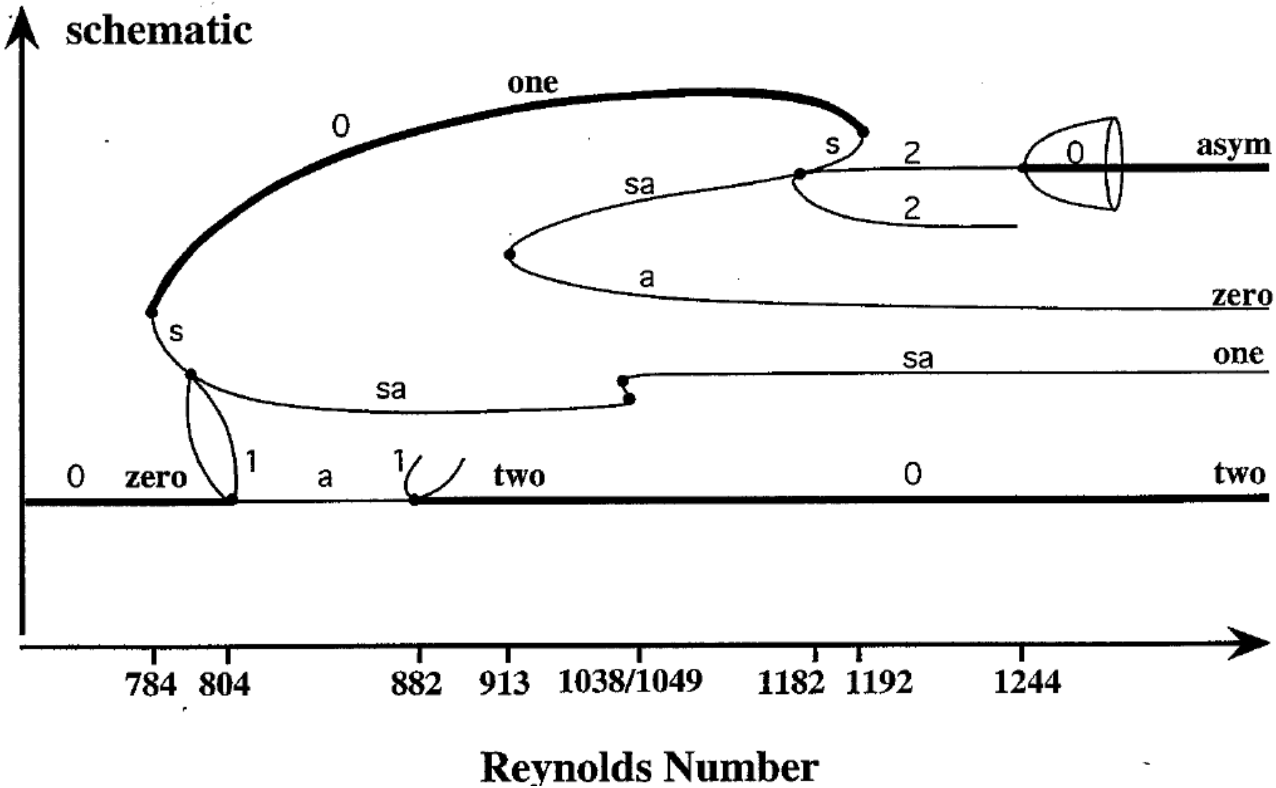
$$\left|\frac{\lambda_2 - s}{\lambda_1 - s}\right| \gg 1 \qquad \text{for } \lambda_1 \approx s$$

AXISYMMETRIC SPHERICAL COUETTE FLOW



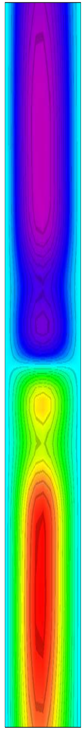

TORQUE VERSUS REYNOLDS NUMBER
250
225
200
175
150
125
Torque
600
800
1000
1200
1400
Reynolds Number
zero(s)
zero(u)
one(s)
one(u)
two(s)
two(u)
asym(s)
asym(u)

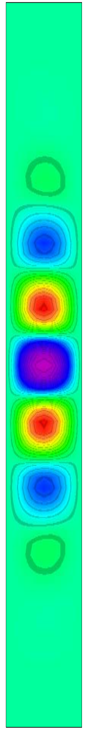
AXISYMMETRIC SPHERICAL COUETTE FLOW



Axisymmetric Spherical Couette Flow

Basic flow at $Re = 650$

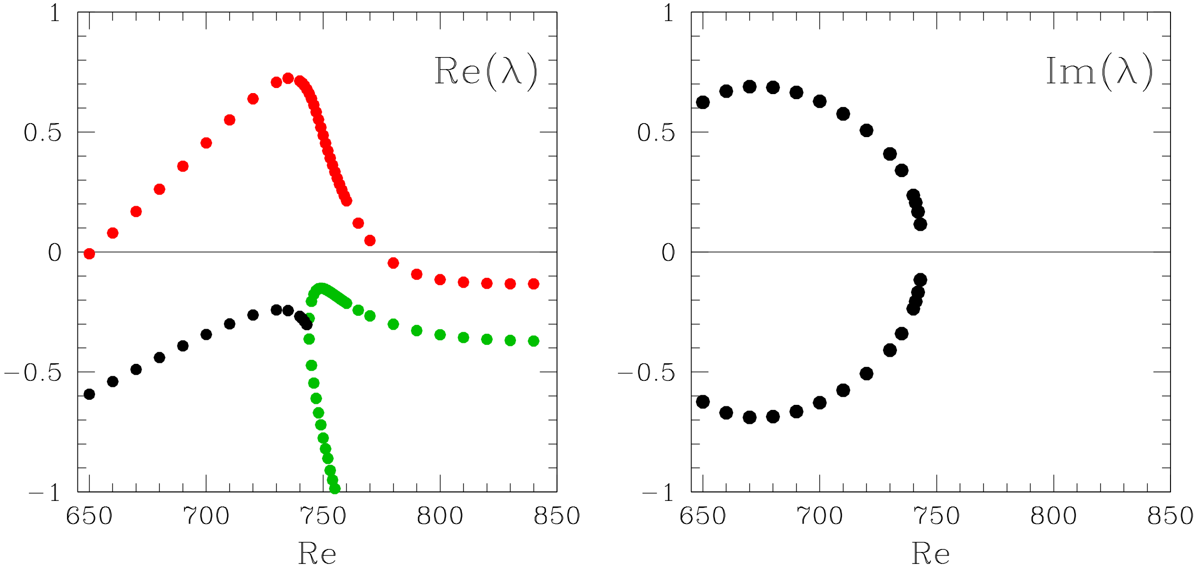




Leading eigenvector

Eigenvalues of Spherical Couette Flow

Obtained from inverse power power method with shift



Bose-Einstein Condensation

Ultra-cold coherent state of matter

Predicted by Bose (1924) and Einstein (1925)

Realized experimentally by Cornell, Ketterle, Wieman (1995)

Nobel prize (2001)

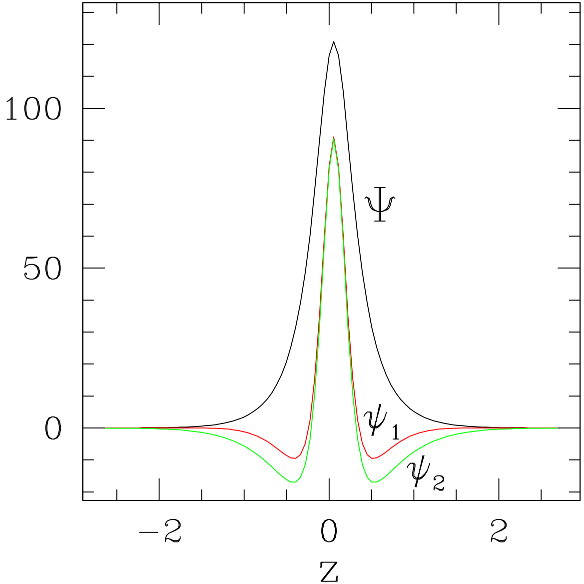
Gross-Pitaevskii / Nonlinear Schrödinger Equation

$$\partial_t \Psi = i\,[\underbrace{\frac{1}{2}\Delta}_{L} + \underbrace{\mu - V(r) - a|\Psi|^2}_{N}]\Psi$$

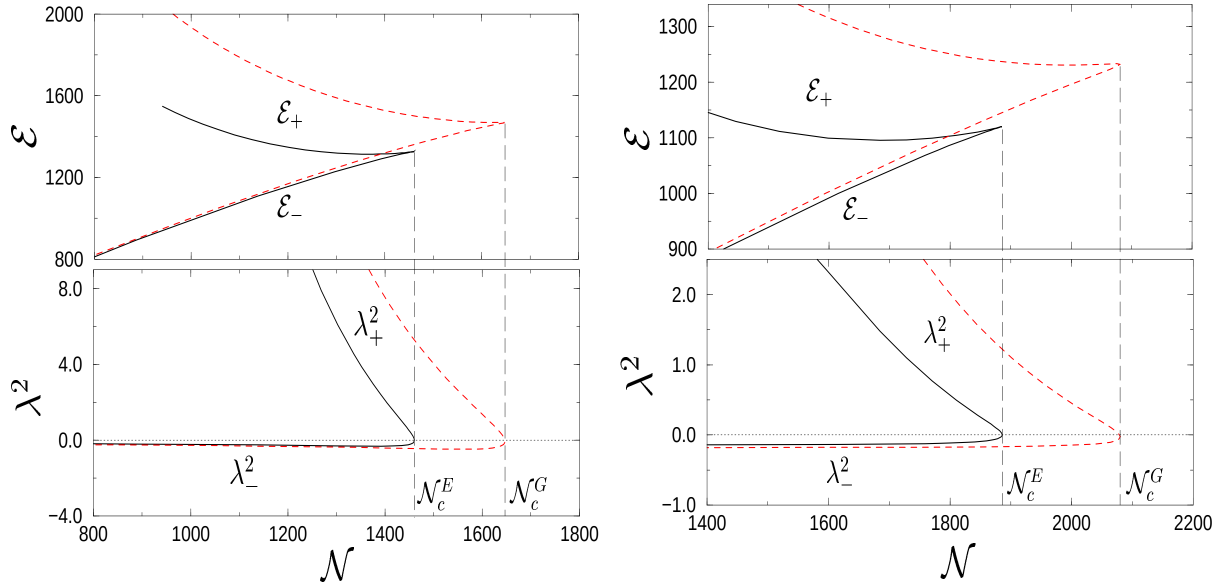
$$V(\mathrm{x}) = \frac{1}{2}|\omega \cdot \mathrm{x}|^2 = \frac{1}{2}(\omega_r r^2 + \omega_z z^2) \qquad \textbf{(cylindrical trap)}$$

Spatial discretisation up to $M = 10^2 \times 10^2 \times 10^2 = 10^6$

Eigenvalues, energies determine decay rates of condensate

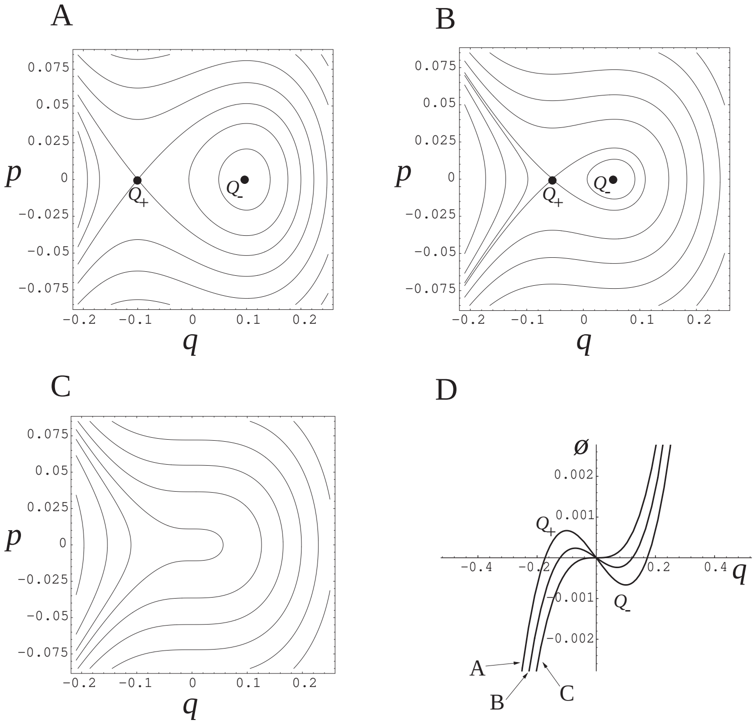


100
50
0
−2
0
2
Z
Ψ
ψ1
ψ2



$\omega_z = \omega_r/5$ **(cigar)** $\omega_r = \omega_z/5$ **(pancake)**

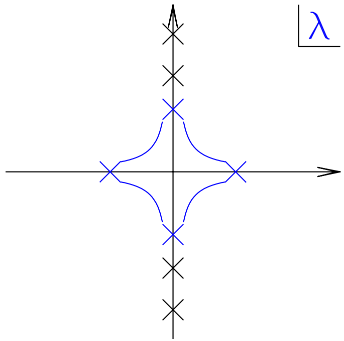
Hamiltonian saddle-node bifurcation of hyperbolic and elliptic fixed points



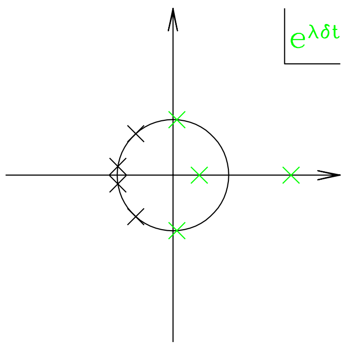
A
B
C
D
p
q
Q+
Q-
0.075
0.05
0.025
0
−0.025
−0.05
−0.075
−0.2
−0.1
0.1
0.2
ø
0.002
0.001
−0.001
−0.002
−0.4
0.4

Hamiltonian Systems

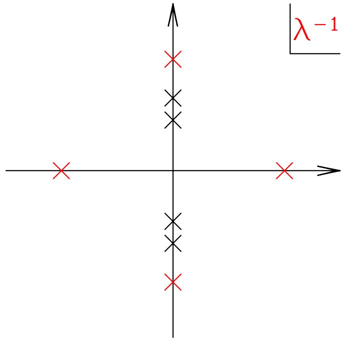
$$f(A) = A$$



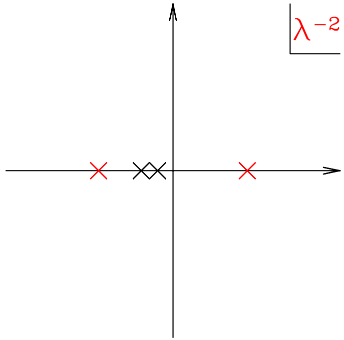
$$f(A) = e^{A\Delta t}$$



$$f(A) = A^{-1}$$



$$f(A) = A^{-2}$$



Steady state solving via Newton's Method:

$$\mathbf{0 = L\Psi + N(\Psi)}$$

Linear stability of steady state $\mathbf{\Psi}$:

$$\partial_t \psi = i\,[(\frac{1}{2}\Delta + \mu - V(r))\psi - a\Psi^2(2\psi + \psi^*)]$$

$$A \begin{pmatrix} \psi^R \\ \psi^I \end{pmatrix} \equiv \begin{bmatrix} 0 & -(L + DN^I) \\ L + DN^R & 0 \end{bmatrix} \begin{pmatrix} \psi^R \\ \psi^I \end{pmatrix}$$

$$\begin{aligned} DN^R &\equiv \mu - V(\mathrm{x}) - 3a\Psi^2 \\ DN^I &\equiv \mu - V(\mathrm{x}) - a\Psi^2 \end{aligned}$$

$$A^2 \begin{pmatrix} \psi^R \\ \psi^I \end{pmatrix} =$$

$$\begin{bmatrix} -(L+DN^I)(L+DN^R) & 0 \\ 0 & -(L+DN^R)(L+DN^I) \end{bmatrix} \begin{pmatrix} \psi^R \\ \psi^I \end{pmatrix}$$

Square, Shift and Invert:

$$(A^2 - s^2 I)\psi_{n+1} = \psi_n$$

Sometimes it is easier to solve a preconditioned version:

$$L^{-2}(A^2 - s^2 I)\psi_{n+1} = L^{-2}\psi_n$$

Floquet theory

Linear equations with constant coefficients:

$$a\ddot{x} + b\dot{x} + cx = 0 \implies x(t) = \alpha_1 e^{\lambda_1 t} + \alpha_2 e^{\lambda_2 t}$$

where $a\lambda^2 + b\lambda + c = 0$

$$\dot{x} = cx \implies x(t) = e^{ct} x(0)$$

$$\sum_{n=0}^{N} c_n x^{(n)} = 0 \implies x(t) = \sum_{n=1}^{N} \alpha_n e^{\lambda_n t}$$

where $\sum_{n=0}^{N} c_n \lambda^n = 0$

Generalize to linear equations with periodic coefficients:

$$a(t)\ddot{x} + b(t)\dot{x} + c(t)x = 0 \implies x(t) = \alpha_1(t) e^{\lambda_1 t} + \alpha_2(t) e^{\lambda_2 t}$$

$a(t), b(t), c(t)$ **have period** T $\implies$ $\alpha_1(t), \alpha_2(t)$ **have period** T

Floquet theory continued

$$a(t)\ddot{x} + b(t)\dot{x} + c(t)x = 0 \Longrightarrow x(t) = \alpha_1(t)e^{\lambda_1 t} + \alpha_2(t)e^{\lambda_2 t}$$

$\alpha_1(t)$, $\alpha_2(t)$	**Floquet functions**
λ_1, λ_2	**Floquet exponents**
$e^{\lambda_1 T}$, $e^{\lambda_2 T}$	**Floquet multipliers**

λ_1, λ_2 not roots of polynomial $\Longrightarrow$ must calculate numerically or asymptotically

$$\dot{x} = c(t)x \implies x(t) = e^{\lambda t}\alpha(t)$$

$$\sum_{n=0}^{N} c_n(t)x^{(n)} = 0 \implies x(t) = \sum_{n=1}^{N} e^{\lambda_n t}\alpha_n(t)$$

Floquet theory and linear stability analysis

Dynamical system: $\dot{x} = f(x)$

Limit cycle solution: $\overline{x}(t+T) = \overline{x}(t)$ **with** $\dot{\overline{x}}(t) = f(\overline{x}(t))$

Stability of $\overline{x}(t)$: $x(t) = \overline{x}(t) + \epsilon(t)$

$$
\begin{aligned}
\dot{\overline{x}} + \dot{\epsilon} &= f(\overline{x}(t)) + f'(\overline{x}(t))\epsilon(t) + \ldots \\
\dot{\epsilon} &= f'(\overline{x}(t))\epsilon(t)
\end{aligned}
$$

Floquet form! $\epsilon(t) = e^{\lambda t}\alpha(t)$ **with $\alpha(t)$ of period T**

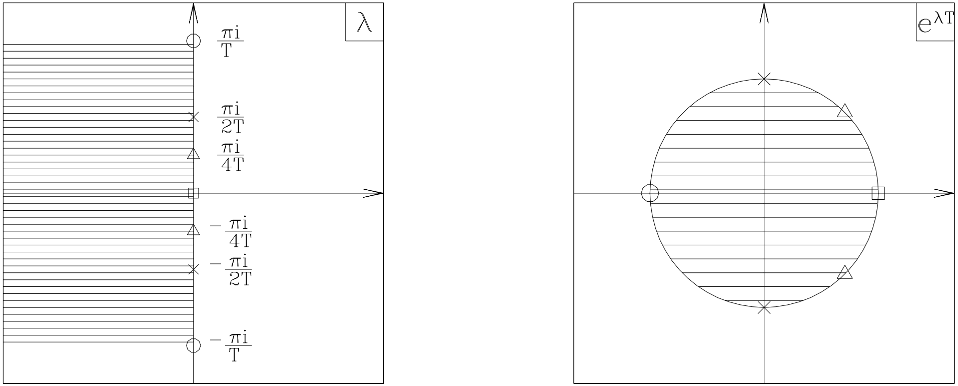
$\mathrm{Re}(\lambda) > 0 \Longrightarrow \overline{x}(t)$ **unstable**

$\mathrm{Re}(\lambda) < 0 \Longrightarrow \overline{x}(t)$ **stable**

λ **complex** $\Longrightarrow$ **most unstable or least stable pert has period different from $\overline{x}(t)$**

Region of stability

for exponent λ **for multiplier $e^{\lambda T}$**



Imaginary part non-unique $\Longrightarrow$ choose Im$(\lambda) \in (-\pi i/T, \pi i/T]$

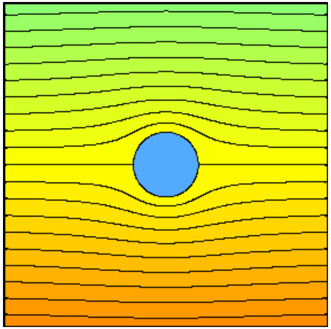
In $\mathcal{R}^N$, $\overline{x}(t)$ stable iff real parts of all λ_j are negative

Monodromy matrix: $\dot{M} = Df(\overline{x}(t))M \quad$ with $M(t=0) = I$

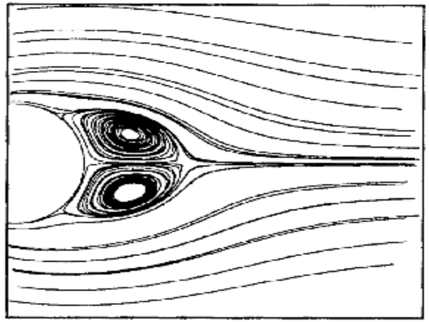
Floquet multipliers/functions = eigenvalues/vectors of $M(T)$

Cylinder wake

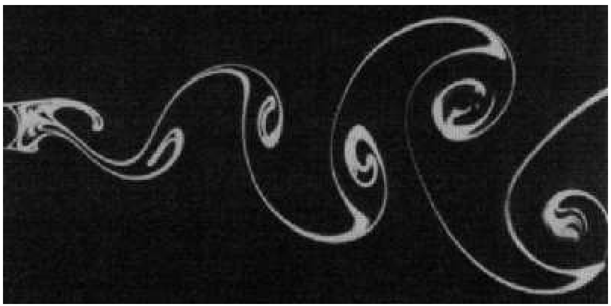
Ideal flow



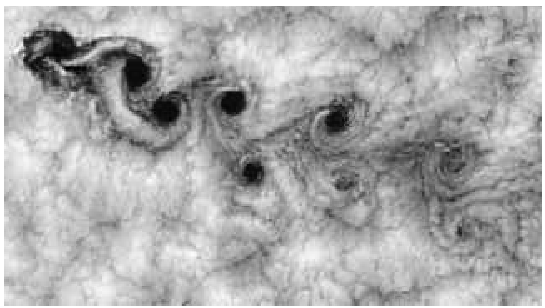
with downstream recirculation zone



Von Kármán vortex street ($\mathrm{Re} \geq 46$)

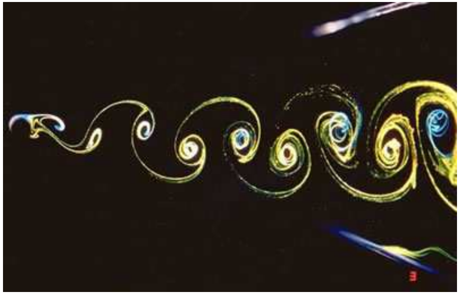


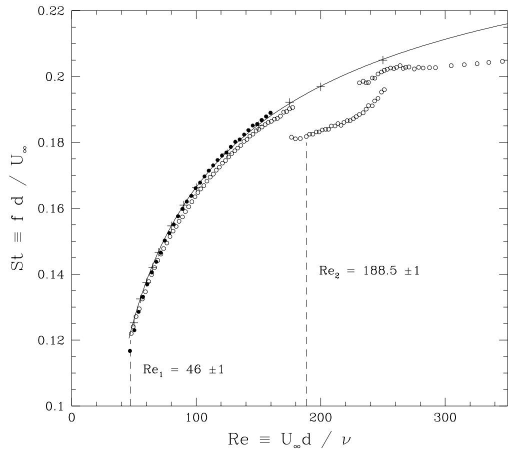
Laboratory experiment (Taneda, 1982)



Off Chilean coast past Juan Fernandez islands

von Kármán vortex street: $Re = U_\infty d/\nu \geq 46$





spatially:
two-dimensional (x, y)
(homogeneous in z)

temporally:
periodic, $St = fd/U_\infty$
appears spontaneously

$$\mathrm{U}_{2D}(x, y, t \bmod T)$$

Stability analysis of von Kármán vortex street

2D limit cycle $\mathrm{U}_{2D}(x, y, t\mathrm{mod}\ T)$ **obeys:**

$$\partial_t \mathrm{U}_{2D} = -(\mathrm{U}_{2D} \cdot \nabla)\mathrm{U}_{2D} - \nabla P_{2D} + \frac{1}{Re}\Delta \mathrm{U}_{2D}$$

Perturbation obeys:

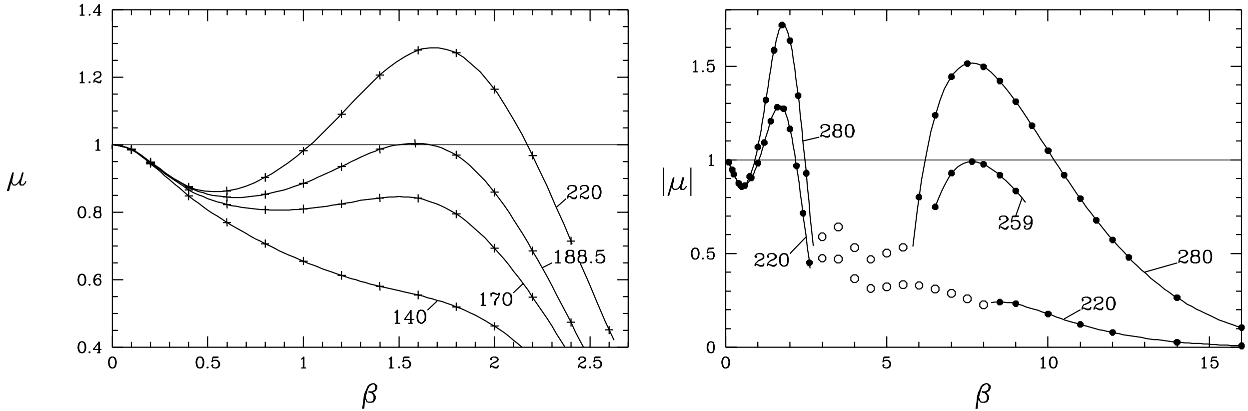
$$\partial_t \mathbf{u}_{3D} = -(\mathrm{U}_{2D}(t) \cdot \nabla)\mathbf{u}_{3D} - (\mathbf{u}_{3D} \cdot \nabla)\mathrm{U}_{2D}(t) - \nabla p_{3D} + \frac{1}{Re}\Delta \mathbf{u}_{3D}$$

Equation homogeneous in z**, periodic in** $t \Longrightarrow$

$$\mathbf{u}_{3D}(x, y, z, t) \sim e^{i\beta z} e^{\lambda_\beta t} \mathrm{f}_\beta(x, y, t \bmod T)$$

Fix β**, calculate largest** $\mu = e^{\lambda_\beta T}$ **via linearized Navier-Stokes**

From Barkley & Henderson, J. Fluid Mech. (1996)



mode A: $\mathbf{Re_c = 188.5}$

$\boldsymbol{\beta}_\mathbf{c} = \mathbf{1.585} \Longrightarrow \boldsymbol{\lambda}_\mathbf{c} \approx \mathbf{4}$

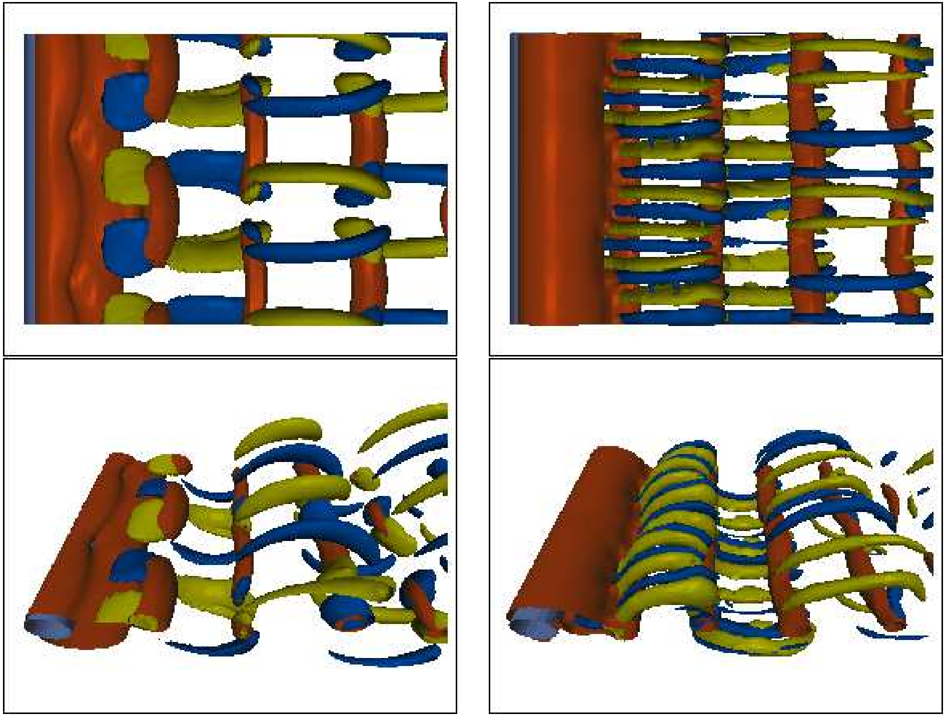
mode B: $\mathbf{Re_c = 259}$

$\boldsymbol{\beta}_\mathbf{c} = \mathbf{7.64} \Longrightarrow \boldsymbol{\lambda}_\mathbf{c} \approx \mathbf{1}$

Temporally: $\mu = 1 \Longrightarrow$
steady bifurcation to limit cycle with same periodicity as U_{2D}

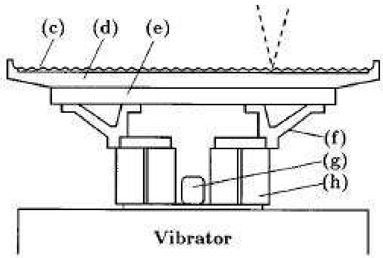
Spatially: circle pitchfork (any phase in z**)**

mode A at $\mathrm{Re} = 210$ **mode B at $\mathrm{Re} = 250$**



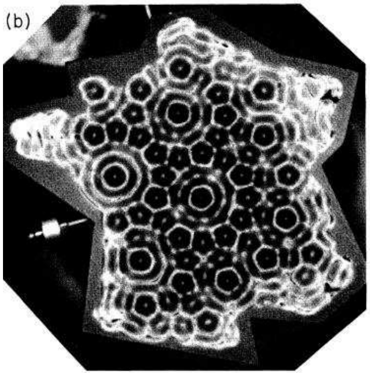
From M.C. Thompson, Monash University, Australia
(http://mec-mail.eng.monash.edu.au/$\sim$mct/mct/docs/cylinder.html)

Faraday instability

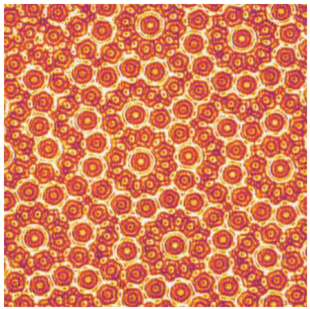


Faraday (1831): Vertical vibration of fluid layer $\Longrightarrow$ stripes, squares, hexagons

In 1990s: first fluid-dynamical quasicrystals:



Edwards & Fauve
J. Fluid Mech. (1994)



Kudrolli, Pier & Gollub
Physica D (1998)

Oscillating frame of reference $\Longrightarrow$ "oscillating gravity"

$$\begin{aligned} G(t) &= g\,(1 - a\cos(\omega t)) \\ G(t) &= g\,(1 - a\,[\cos(m\omega t) + \delta\cos(n\omega t + \phi_0)]) \end{aligned}$$

Flat surface becomes linearly unstable for sufficiently high a

Consider domain to be horizontally infinite (homogeneous) $\Longrightarrow$ solutions exponential/trigonometric in $\mathrm{x} = (x, y)$

Seek bounded solutions $\Longrightarrow$ trigonometric: $\exp(i\mathrm{k}\cdot\mathrm{x})$

$$\textbf{Height}\ \ \zeta(x, y, t) = \sum_{\mathrm{k}} e^{i\mathrm{k}\cdot\mathrm{x}}\hat{\zeta}_k(t)$$

Oscillating gravity $\Longrightarrow$ temporal Floquet problem, $T = 2\pi/\omega$

$$\hat{\zeta}_k(t) = \sum_j e^{\lambda_k^j t} f_k^j(t)$$

$$\text{Height } \zeta(x,y,t) = \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{x}} \hat{\zeta}_k(t)$$

Ideal fluids (no viscosity), sinusoidal forcing $\Longrightarrow$ Mathieu eq.

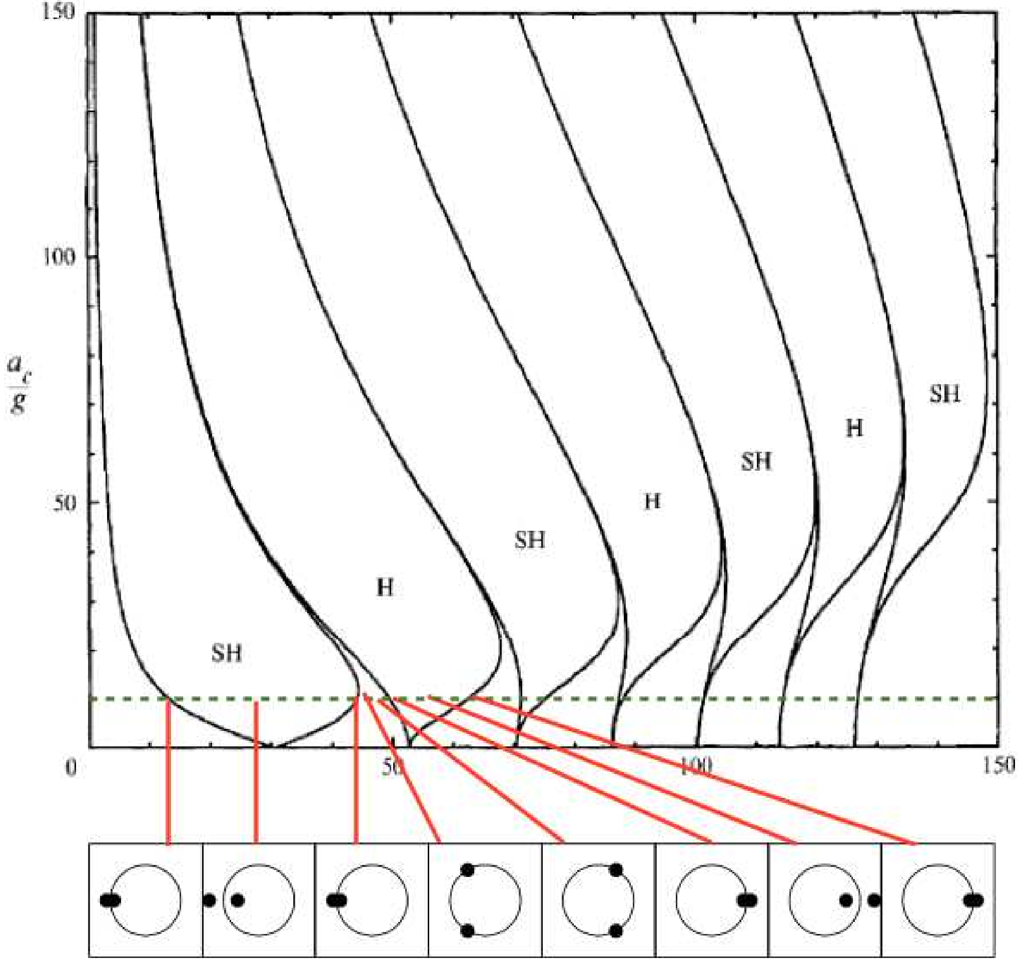
$$\partial_t^2 \hat{\zeta}_k + \omega_0^2 \left[1 - a\cos(\omega t)\right] \hat{\zeta}_k = 0$$

ω_0^2 **combines g, densities, surface tension, wavenumber k**

$$\hat{\zeta}_k(t) = \sum_{j=1}^{2} e^{\lambda_k^j t} f_k^j(t)$$

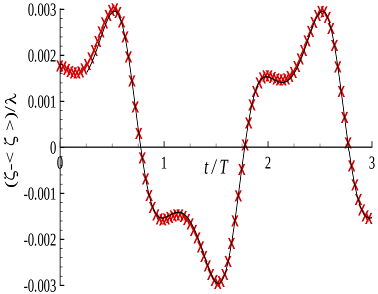
Re$(\lambda_k^j) > 0$ for some $j, k \Longrightarrow \hat{\zeta}_k \nearrow \Longrightarrow$ flat surface unstable
$\Longrightarrow$ Faraday waves with wavelength $2\pi/k$

Im(λ_k^j)	$e^{\lambda T}$	**waves**	**period**
0	**1**	**harmonic**	**same as forcing**
$\omega/2$	-1	**subharmonic**	**twice forcing period**

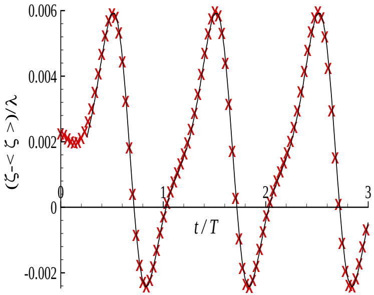


150
100
50
0
50
100
150
$\frac{a_c}{g}$
SH
H
SH
H
SH
H
SH

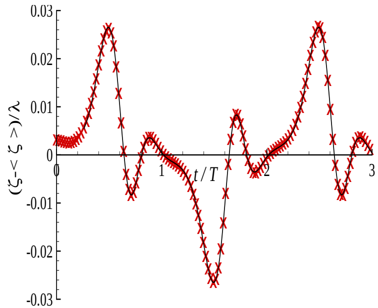
Floquet functions



within tongue 1 /2
subharmonic
$\mu = -1$



within tongue 2 /2
harmonic
$\mu = +1$



within tongue 3 /2
subharmonic
$\mu = -1$

Hexagonal patterns in Faraday instability