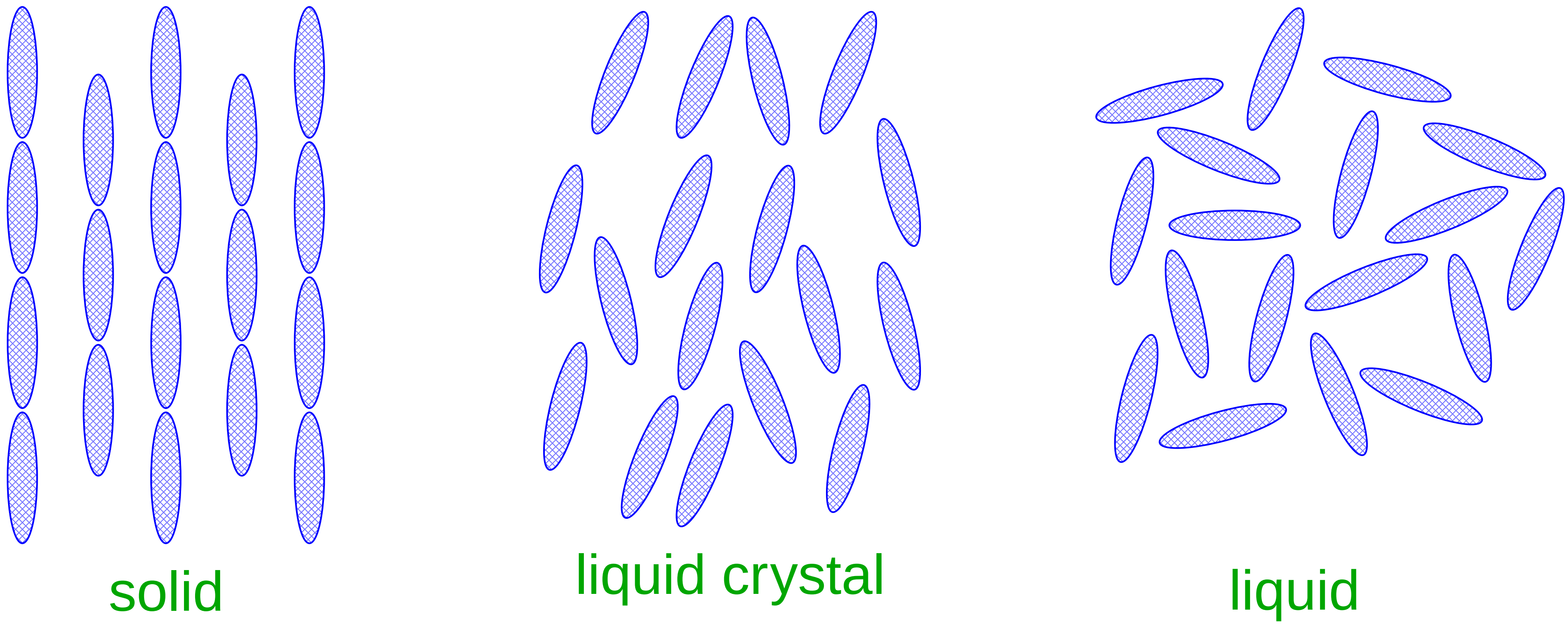
Saddle point problems in liquid crystal modelling

Alison Ramage
Dept of Mathematics
University of Strathclyde
Glasgow, Scotland

Eugene C. Gartland, Jr.
Dept of Mathematics
Kent State University
Ohio, USA

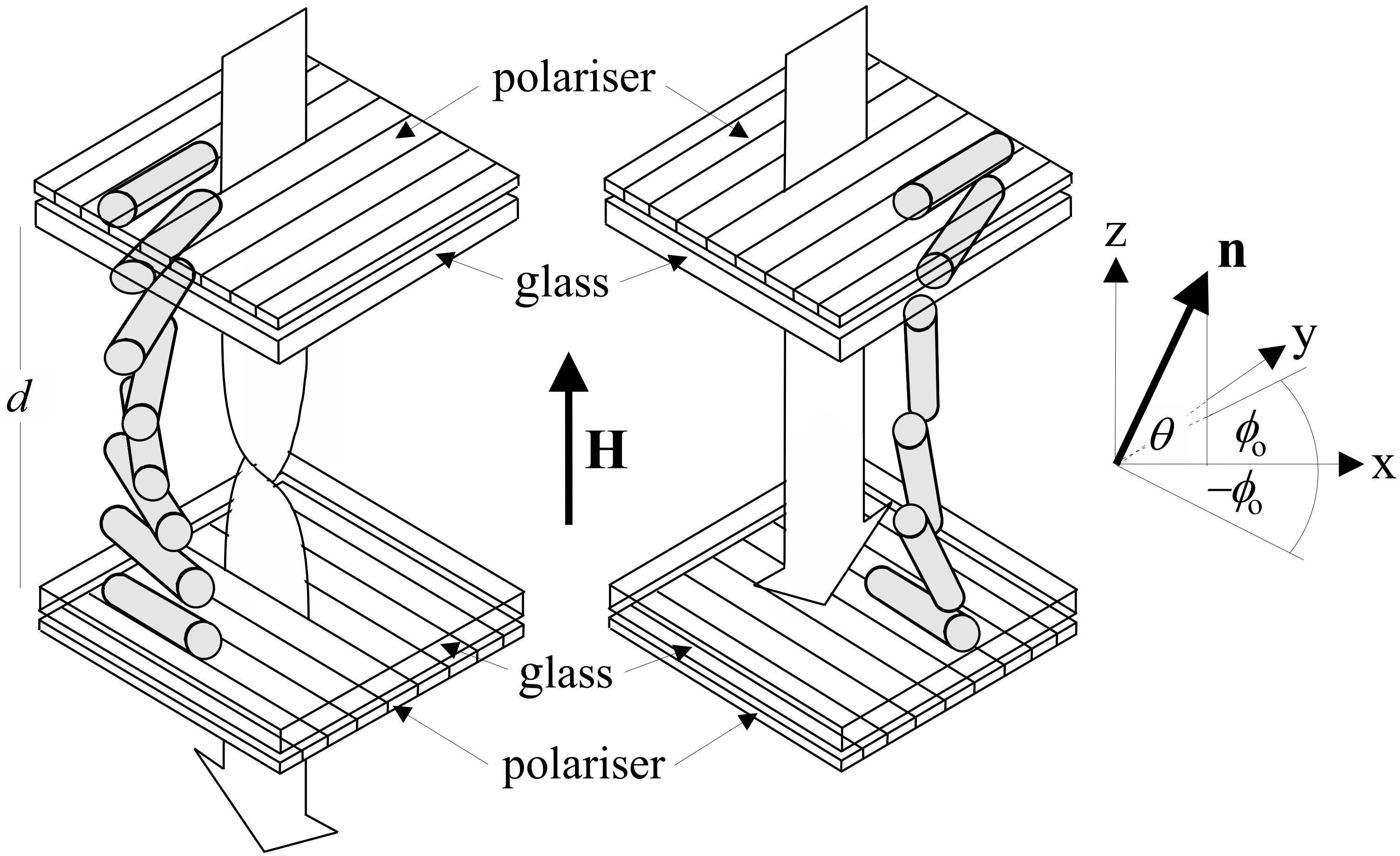
Liquid Crystals

- occur between solid crystal and isotropic liquid states



- may have different equilibrium configurations
- switch between stable states by altering applied voltage, magnetic field, boundary conditions, ...

Liquid Crystal Displays

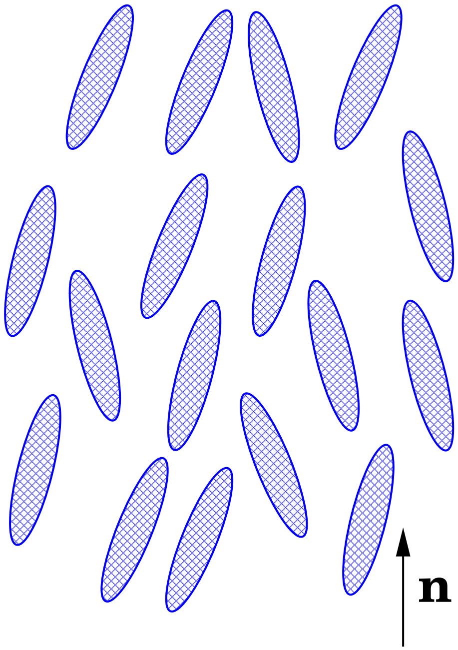


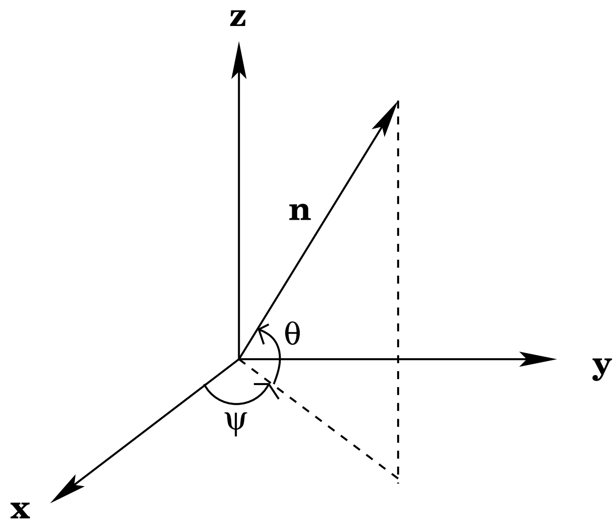
(a) 'off state' $H < H_c$ (b) 'on state' $H > H_c$

twisted nematic device

Static and Dynamic Continuum Theory of Liquid Crystals,
Iain W. Stewart (2004)

Modelling: Director-based models





- director: average direction of molecular alignment

  unit vector $\mathbf{n} = (\cos\theta\cos\psi, \cos\theta\sin\psi, \sin\theta)$

- order parameter: measure of orientational order

$$S = \frac{1}{2} < 3\cos^2\theta_m - 1 >$$

Finding Equilibrium Configurations

- minimise the free energy density

$$\mathcal{F} = \int_V F_{bulk}(\theta, \psi, \nabla\theta, \nabla\psi) + \int_{\mathcal{S}} F_{surface}(\theta, \phi)\, d\mathcal{S}$$

$$F_{bulk} = F_{elastic} + F_{electrostatic}$$

- if fixed boundary conditions are applied, surface energy term can be ignored

- solutions with least energy are physically relevant

- use calculus of variations: Euler-Lagrange equations

Elastic Energy

- Frank-Oseen elastic energy

$$
\begin{aligned}
F_{elastic} &= \frac{1}{2}K_1(\nabla\cdot\mathbf{n})^2 + \frac{1}{2}K_2(\mathbf{n}\cdot\nabla\times\mathbf{n})^2 \\
&+ \frac{1}{2}K_3(\mathbf{n}\times\nabla\times\mathbf{n})^2 \\
&+ \frac{1}{2}(K_2+K_4)\nabla\cdot[(\mathbf{n}\cdot\nabla)\mathbf{n}-(\nabla\cdot\mathbf{n})\mathbf{n}]
\end{aligned}
$$

- Frank elastic constants

K_1	splay
K_2	twist
K_3	bend
$K_2 + K_4$	saddle-splay

One-Constant Approximation

- set

$$K = K_1 = K_2 = K_3, \qquad K_4 = 0$$

- vector identities

$$(\nabla \times \mathbf{n})^2 = (\mathbf{n} \cdot \nabla \times \mathbf{n})^2 + (\mathbf{n} \times \nabla \times \mathbf{n})^2$$

$$\nabla(\mathbf{n} \cdot \mathbf{n}) = 0$$

$$\left[(\nabla \cdot \mathbf{n})^2 + (\nabla \times \mathbf{n})^2\right] + \nabla \cdot \left[(\mathbf{n} \cdot \nabla)\mathbf{n} - (\nabla \cdot \mathbf{n})\mathbf{n}\right] = \|\nabla \mathbf{n}\|^2$$

- elastic energy $\quad F_{elastic} = \frac{1}{2} K \|\nabla \mathbf{n}\|^2$

Electrostatic Energy

- applied electric field $\mathbf{E}$ of magnitude E

- electrostatic energy

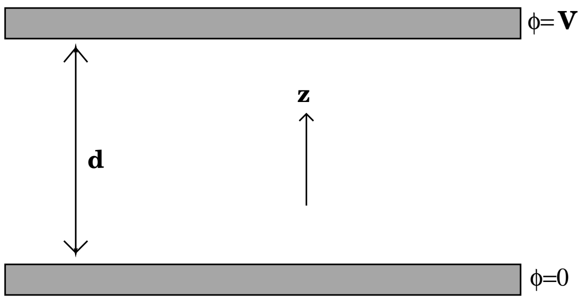
$$F_{electrostatic} = -\frac{1}{2}\epsilon_0 \epsilon_\perp E^2 - \frac{1}{2}\epsilon_0 \epsilon_a (\mathbf{n}\cdot\mathbf{E})^2$$

- dielectric anisotropy $\epsilon_a = \epsilon_\parallel - \epsilon_\perp$

- permittivity of free space ϵ_0

Model Problem: Twisted Nematic Device

- two parallel plates distance d apart



- strong anchoring parallel to plate surfaces ($\mathbf{n}$ fixed)

- rotate one plate through $\pi/2$ radians

- electric field $\mathbf{E} = (0, 0, E(z))$,   voltage V

Equilibrium Equations 1

- equilibrium equations on $z \in [0, d]$

$$F = \frac{1}{2} \int_0^d \left\{ K \|\nabla \mathbf{n}\|^2 - \epsilon_0 \epsilon_\perp E^2 - \epsilon_0 \epsilon_a (\mathbf{n} \cdot \mathbf{E})^2 \right\} dz$$

- director $\mathbf{n} = (u, v, w)$, $|\mathbf{n}| = 1$
- constraint applied via Lagrange multipliers λ
- electric potential ϕ: $E = \dfrac{d\phi}{dz}$
- unknowns u, v, w, ϕ, λ

Equilibrium Equations 2

- nondimensionalised equilibrium equations on $z \in [0,1]$

$$\begin{aligned} F &= \frac{1}{2}\int_0^1 \left[(u_z^2 + v_z^2 + w_z^2) - \alpha^2 \pi^2 (\beta + w^2) \phi_z^2 \right. \\ &- \left. \lambda (u^2 + v^2 + w^2 - 1) \right] \, dz \end{aligned}$$

- dimensionless parameters

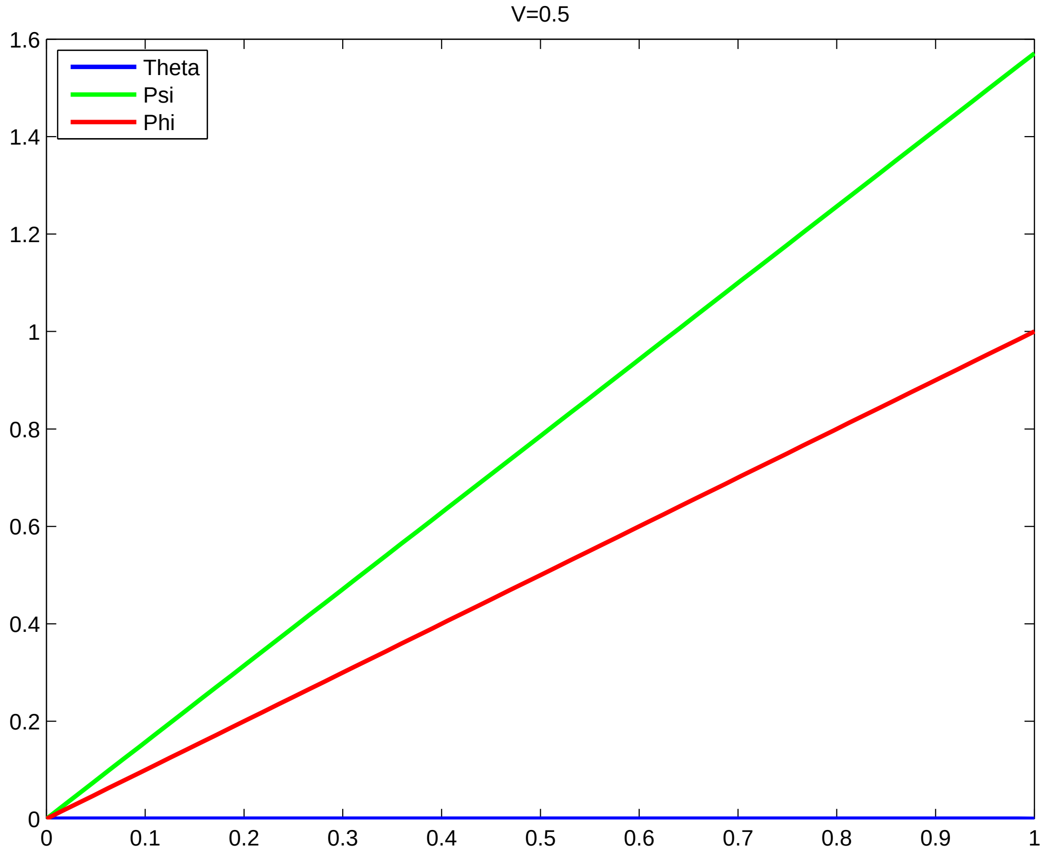
$$\alpha^2 = \frac{\epsilon_0 \epsilon_a V^2}{K \pi^2}, \qquad \beta = \frac{\epsilon_\perp}{\epsilon_a}$$

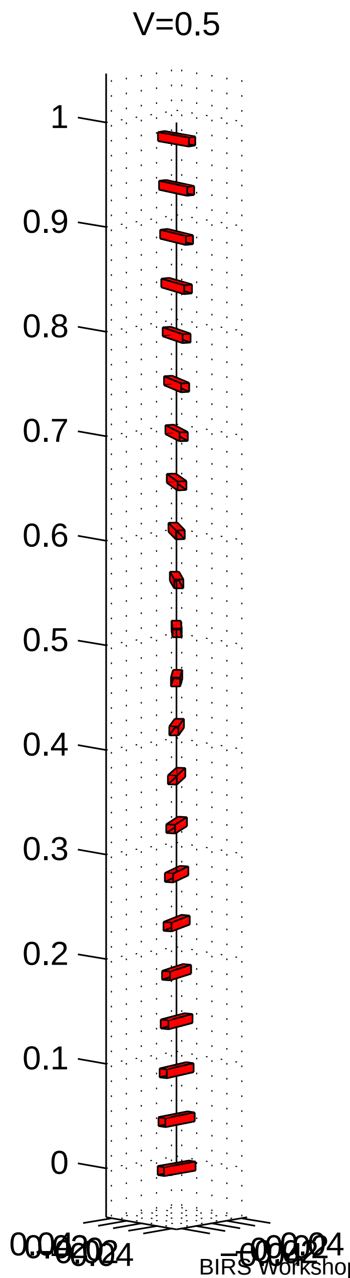
- boundary conditions:

at $z = 0$: $\theta = \psi = \phi = 0$, at $z = 1$: $\theta = 0$, $\psi = \dfrac{\pi}{2}$, $\phi = 1$

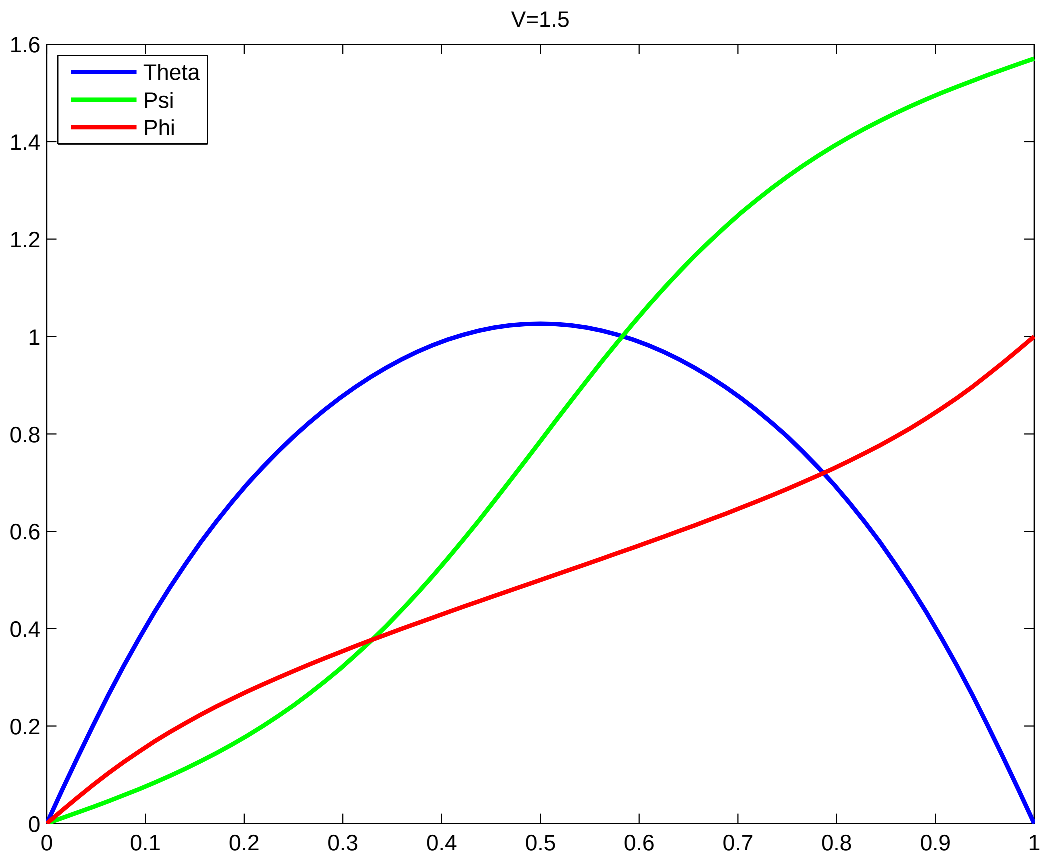
Off State

$$\theta(z) \equiv 0, \qquad \psi(z) = \frac{\pi z}{2}, \qquad \phi(z) = z$$

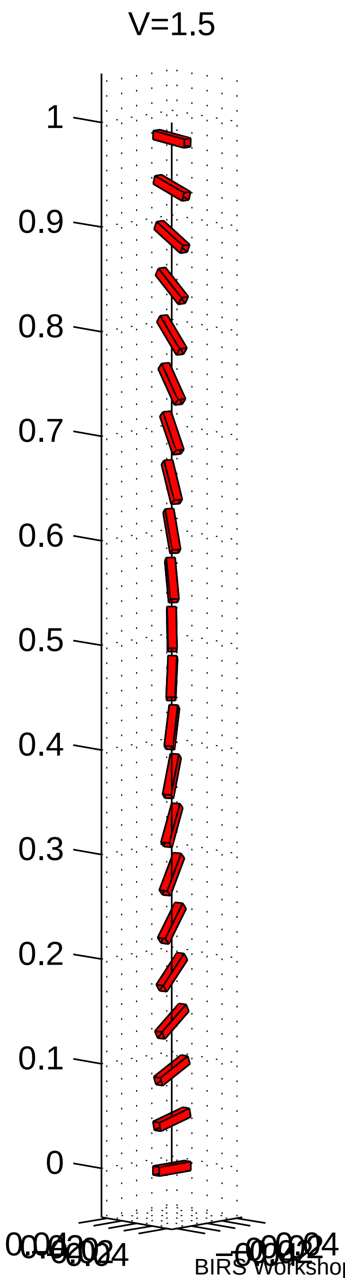




On State



V=1.5
Theta
Psi
Phi
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

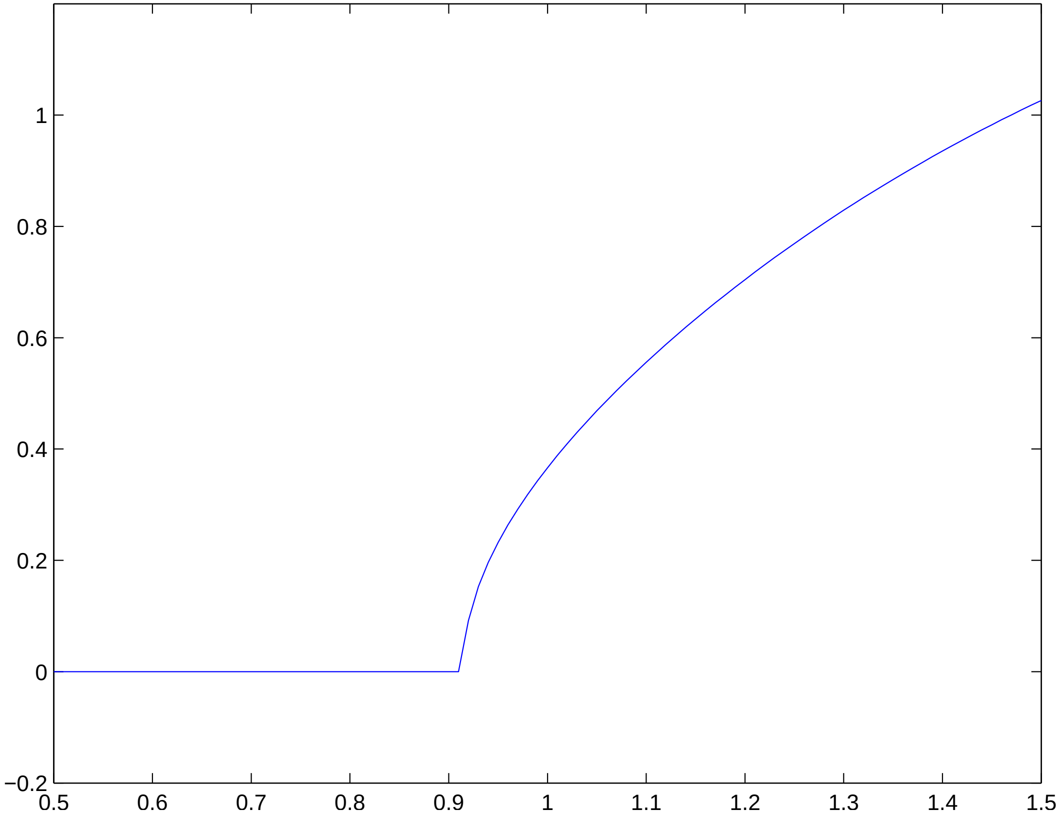


V=1.5
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0

Critical Voltage

- switching occurs at

$$V_c = \frac{\pi}{2}\sqrt{\frac{3K}{\epsilon_0 \epsilon_a}}$$



Discrete Free Energy

- grid of $N+1$ points z_k a distance Δz apart
- approximate integral by mid-point rule

$$
\begin{aligned}
F \;\simeq\; & \frac{\Delta z}{2} \sum_{k=0}^{N-1} \left\{ \left[\frac{u_{k+1} - u_k}{\Delta z} \right]^2 + \left[\frac{v_{k+1} - v_k}{\Delta z} \right]^2 + \left[\frac{w_{k+1} - w_k}{\Delta z} \right]^2 \right. \\
- \; & \alpha^2 \pi^2 \left(\beta + \left[\frac{w_k^2 + w_{k+1}^2}{2} \right] \right) \left[\frac{\phi_{k+1} - \phi_k}{\Delta z} \right]^2 \\
- \; & \left. \lambda_k \left[\frac{u_k^2 + u_{k+1}^2}{2} + \frac{v_k^2 + v_{k+1}^2}{2} + \frac{w_k^2 + w_{k+1}^2}{2} - 1 \right] \right\}
\end{aligned}
$$

Euler-Lagrange Equations

- set $\dfrac{\partial F}{\partial u_k}, \dfrac{\partial F}{\partial v_k}, \dfrac{\partial F}{\partial w_k}, \dfrac{\partial F}{\partial \phi_k}, \dfrac{\partial F}{\partial \lambda_k}$ equal to zero

- solve $\nabla \mathbf{F}(\mathbf{x}) = \mathbf{0}$ for $\mathbf{x} = [\mathbf{u}, \mathbf{v}, \mathbf{w}, \phi, \lambda]$

  $N+1$ gridpoints $\Rightarrow n = N-1$ unknowns

- use Newton's method: solve

$$\nabla^2 \mathbf{F}(\mathbf{x}_j) \cdot \delta \mathbf{x}_j = -\nabla \mathbf{F}(\mathbf{x}_j)$$

- linear system, coefficient matrix is Hessian $\nabla^2 \mathbf{F}(\mathbf{x}_j)$

$$\nabla^2 \mathbf{F} = \begin{bmatrix} \nabla^2_{\mathbf{nn}} \mathbf{F} & \nabla^2_{\mathbf{n}\phi} \mathbf{F} & \nabla^2_{\mathbf{n}\lambda} \mathbf{F} \\ \nabla^2_{\phi\mathbf{n}} \mathbf{F} & \nabla^2_{\phi\phi} \mathbf{F} & \nabla^2_{\phi\lambda} \mathbf{F} \\ \nabla^2_{\lambda\mathbf{n}} \mathbf{F} & \nabla^2_{\lambda\phi} \mathbf{F} & \nabla^2_{\lambda\lambda} \mathbf{F} \end{bmatrix}$$

Hessian Components 1

- matrix notation: $\nabla^2_{\mathbf{nn}}\mathbf{F} = A$

$$A = \begin{bmatrix} \nabla^2_{\mathbf{uu}}\mathbf{F} & 0 & 0 \\ 0 & \nabla^2_{\mathbf{vv}}\mathbf{F} & 0 \\ 0 & 0 & \nabla^2_{\mathbf{ww}}\mathbf{F} \end{bmatrix} = \begin{bmatrix} A_{uu} & 0 & 0 \\ 0 & A_{vv} & 0 \\ 0 & 0 & A_{ww} \end{bmatrix}$$

- A_{uu}, A_{vv} and A_{ww} are $n \times n$ symmetric tridiagonal blocks
- $A_{uu} = A_{vv} = \dfrac{1}{\Delta z}\texttt{tridiag}(-1, 2 - \Delta z^2 \lambda_j, -1)$
- $A_{ww} = \dfrac{1}{\Delta z}\texttt{tridiag}(-1, 2 - \Delta z^2 \lambda_j - \gamma_j, -1)$

$$\gamma_j = \frac{\alpha^2 \pi^2}{2}[(\phi_{j+1} - \phi_j)^2 + (\phi_j - \phi_{j-1})^2]$$

Eigenvalues of A

- at first Newton step (initial linear ϕ, $\lambda_j = 1$) block matrices are Toeplitz
- find eigenvalues using Fourier analysis
- $\sigma_{\min}(A_{uu}) = \sigma_{\min}(A_{vv}) \simeq \Delta z(\pi^2 - \lambda_1) > 0$

  A_{uu} and A_{vv} are initially positive definite
- $\sigma_{\min}(A_{ww}) \simeq \Delta z(\pi^2(1 - \alpha^2) - \lambda_1)$

  A_{ww} is initially positive definite iff $V < \frac{2}{\sqrt{3}} V_c$
- at subsequent Newton iterations, A_{uu}, A_{vv}, A_{ww} may all be indefinite
- number of negative eigenvalues increases with V

Hessian Components 2

- matrix notation: $\nabla^2_{\mathbf{n}\lambda}\mathbf{F} = B$

- the $3n \times n$ matrix B has structure

$$B = \Delta z \begin{bmatrix} B_u \\ B_v \\ B_w \end{bmatrix}, \qquad \begin{array}{l} B_u = \mathtt{diag}(\mathbf{u}) \\ B_v = \mathtt{diag}(\mathbf{v}) \\ B_w = \mathtt{diag}(\mathbf{w}) \end{array}$$

- $\mathrm{rank}(B^T) = n$

- $B^T B = \Delta z^2 I_n$

- information available about basis for nullspace of B^T

Hessian Components 3

- matrix notation: $\nabla^2_{\phi\phi}\mathbf{F} = -C$
- the $n \times n$ matrix C is symmetric and tridiagonal
- $C = \dfrac{1}{\Delta z}\texttt{tridiag}(-a_{j-\frac{1}{2}}, a_{j-\frac{1}{2}} + a_{j+\frac{1}{2}}, -a_{j+\frac{1}{2}})$

$$a_{j-\frac{1}{2}} = \alpha^2\pi^2(\beta + \frac{1}{2}(w_{j-1}^2 + w_j^2)) > 0$$

$$a_{j+\frac{1}{2}} = \alpha^2\pi^2(\beta + \frac{1}{2}(w_j^2 + w_{j+1}^2)) > 0$$

- diagonally dominant with positive real diagonal entries

C is positive definite

Hessian Components 4

- matrix notation: $\nabla^2_{\mathbf{n}\phi}\mathbf{F} = D$

$$D = \Delta z \begin{bmatrix} 0 \\ 0 \\ \mu D_w \end{bmatrix}, \qquad \mu = \frac{\alpha^2\pi^2}{\Delta z}$$

- the $n \times n$ matrix D_w is tridiagonal

$$D_w = \texttt{diag}(\mathbf{w})\texttt{tridiag}(\phi_j - \phi_{j-1}, \phi_{j-1} - 2\phi_j + \phi_{j+1}, \phi_j - \phi_{j+1}$$

- D_w has complex eigenvalues (including one zero)

- $\mathrm{rank}(D) = n - 1$

Four Saddle-Point Problems

- for unknown vector ordered as $\mathbf{x} = [\mathbf{u}, \mathbf{v}, \mathbf{w}, \phi, \lambda]$

$$H = \left[\begin{array}{c|cc} A & D & B \\ \hline D^T & -C & 0 \\ B^T & 0 & 0 \end{array}\right] \qquad H = \left[\begin{array}{cc|c} A & D & B \\ D^T & -C & 0 \\ \hline B^T & 0 & 0 \end{array}\right]$$

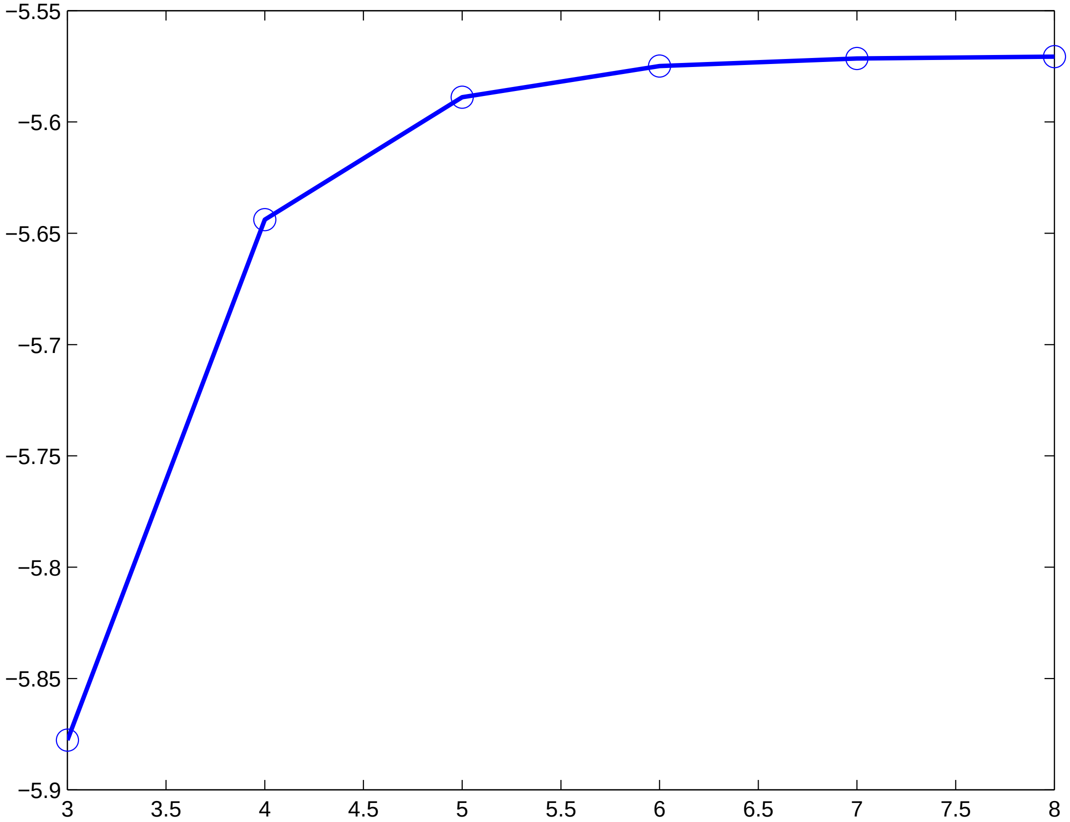
- for unknown vector ordered as $\mathbf{x} = [\mathbf{u}, \mathbf{v}, \mathbf{w}, \lambda, \phi]$

$$H = \left[\begin{array}{c|cc} A & B & D \\ \hline B^T & 0 & 0 \\ D^T & 0 & -C \end{array}\right] \qquad H = \left[\begin{array}{cc|c} A & B & D \\ B^T & 0 & 0 \\ \hline D^T & 0 & -C \end{array}\right]$$

double saddle-point structure

Iterative Solution

- outer iteration: Newton's method tol=$1e-4$
- inner iteration: MINRES tol=$1e-4$
- check accuracy by calculating energy of final solution



Matrix Conditioning

- eigenvalues of H lie in $[\lambda_{\min}, \lambda_s] \cup [\lambda_{s+1}, \lambda_{\max}]$
- estimate of matrix conditioning:

N	`condest`	$\lambda_{\min}(H)$	$\lambda_s(H)$	$\lambda_{s+1}(H)$	$\lambda_{\max}(H)$
8	1.64e+6	-6.68e+2	-5.40e-4	1.88e-1	3.07e+1
16	2.58e+7	-1.44e+3	-6.26e-5	2.19e-1	6.33e+1
32	4.09e+8	-2.98e+3	-7.68e-6	1.28e-1	1.28e+2
64	6.51e+9	-6.07e+3	-9.56e-7	6.60e-2	2.56e+2
128	1.04e+11	-1.23e+4	-1.20e-7	3.33e-2	5.12e+2
256	1.66e+12	-2.46e+4	-1.50e-8	1.67e-2	1.03e+3
	$O(N^4)$	$O(N)$	$O(N^{-3})$	$O(N^{-1})$	$O(N)$

Diagonal Preconditioning

$$H = \begin{bmatrix} A & D & B \\ D^T & -C & 0 \\ B^T & 0 & 0 \end{bmatrix}$$

$$\mathcal{D} = \begin{bmatrix} D_A & 0 & 0 \\ 0 & D_C & 0 \\ 0 & 0 & \Delta z\, I \end{bmatrix} \qquad \begin{aligned} D_A &= |\mathtt{diag}(A)| \\ D_C &= \mathtt{diag}(C) \end{aligned}$$

- estimated condition of $P^{-1}H$ is $O(N^2)$

$$\lambda_{\min} = -2,\ \ \lambda_s = O(N^{-2}),\ \ \lambda_{s+1} = O(N^{-2}),\ \ \lambda_{\max} = 2.$$

Constraint-type Preconditioning

$$H = \left[\begin{array}{cc|c} A & B & D \\ B^T & 0 & 0 \\ \hline D^T & 0 & -C \end{array}\right]$$

$$C_1 = \left[\begin{array}{cc|c} D_A & 0 & D \\ 0 & \Delta z I & 0 \\ \hline D^T & 0 & -C \end{array}\right], \qquad C_2 = \left[\begin{array}{cc|c} A & 0 & D \\ 0 & \Delta z I & 0 \\ \hline D^T & 0 & -C \end{array}\right]$$

- Projected Preconditioned Conjugate Gradients
  Dollar et al. (2006)

Iteration Counts

- iteration counts at first Newton step

N	8	16	32	64	128	256
$\mathcal{D}$	15	40	117	382	1293	5126
C_1	13	25	50	98	195	387
C_2	7	9	8	9	7	8

- iteration counts at last Newton step

N	8	16	32	64	128	256
$\mathcal{D}$	37	134	414	1617	7466	34755
C_1	22	55	226	635	2259	7166
C_2	6	14	23	43	65	114

Other methods?

- block tridiagonal?
- more sophisticated constraint preconditioning?
- Schur complement approximation?
- augmented Lagrangian methods?
- inner/outer iteration?
- connection with harmonic maps?