Saddle point problems in liquid crystal modelling

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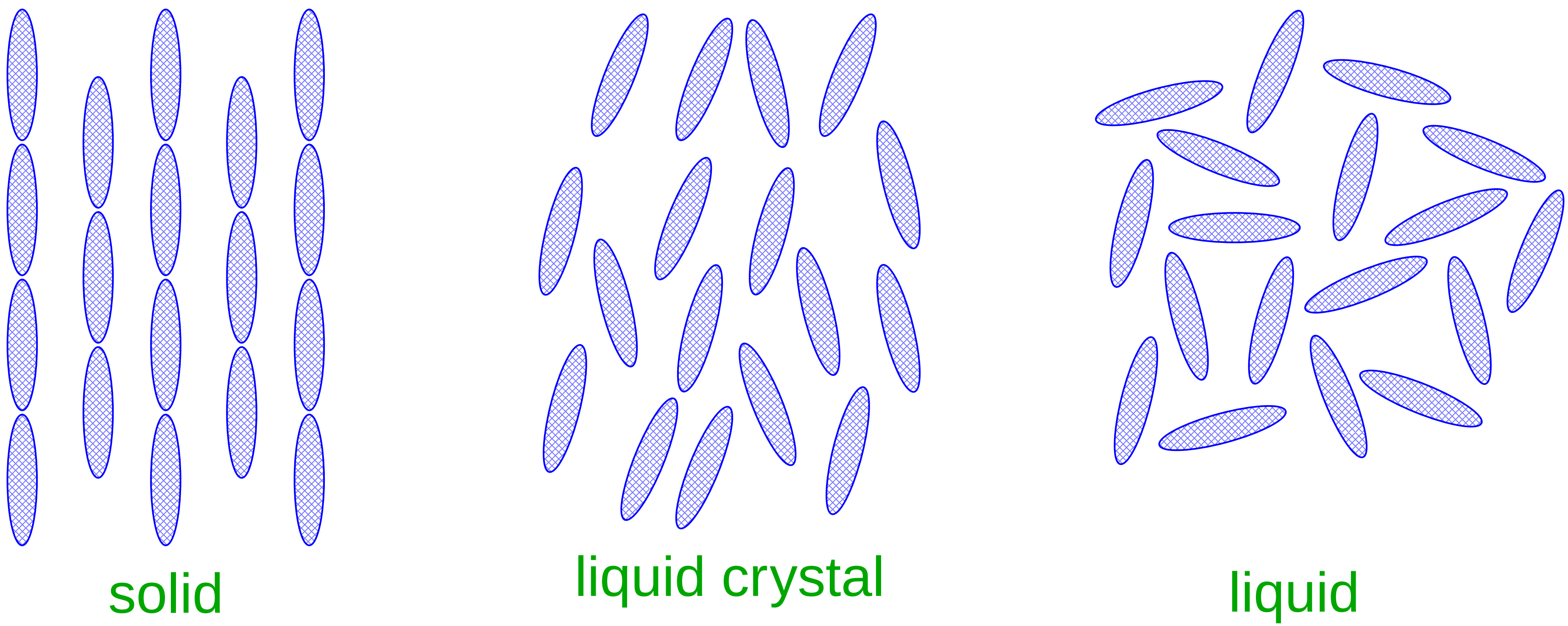
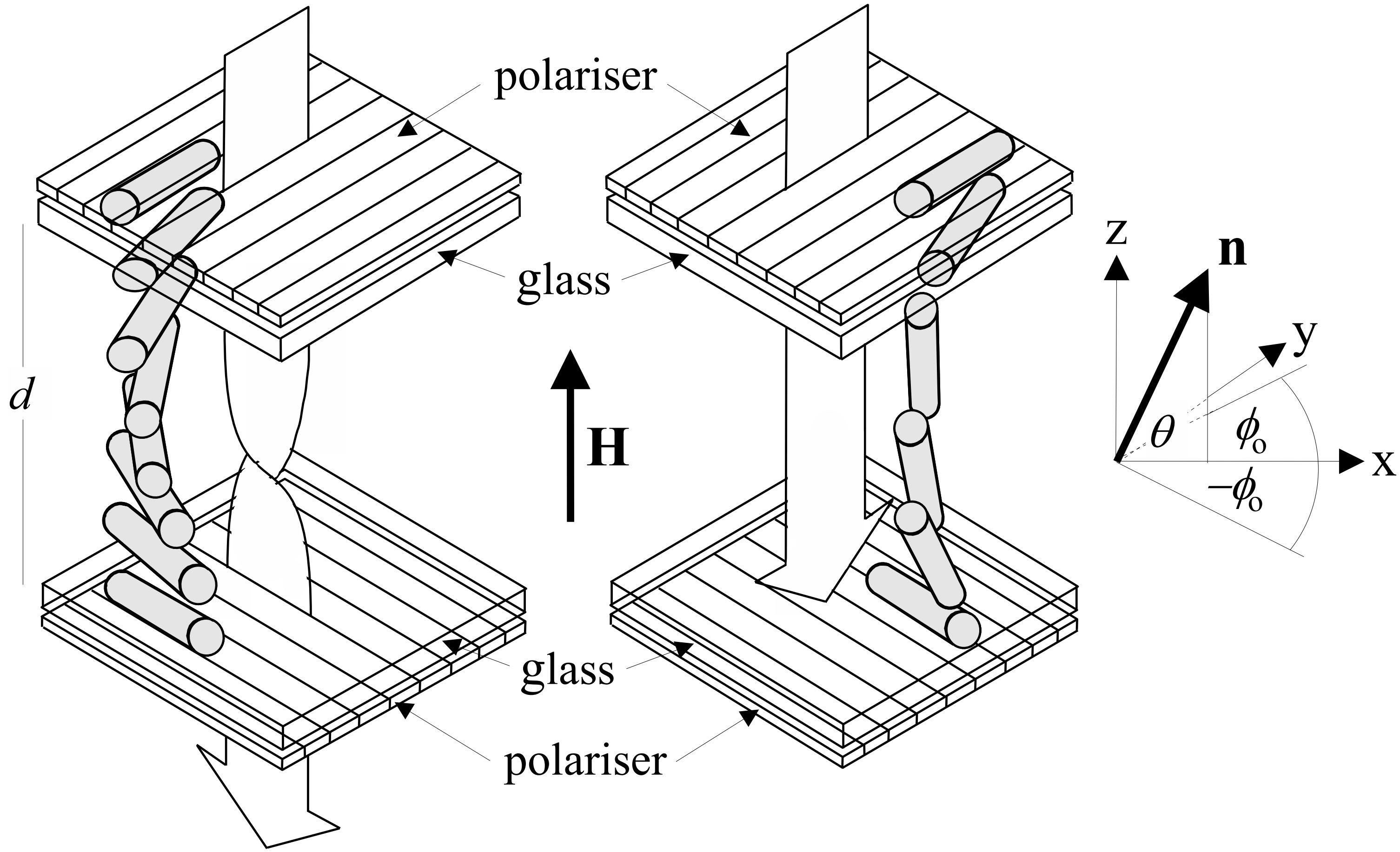
Liquid Crystals

- 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

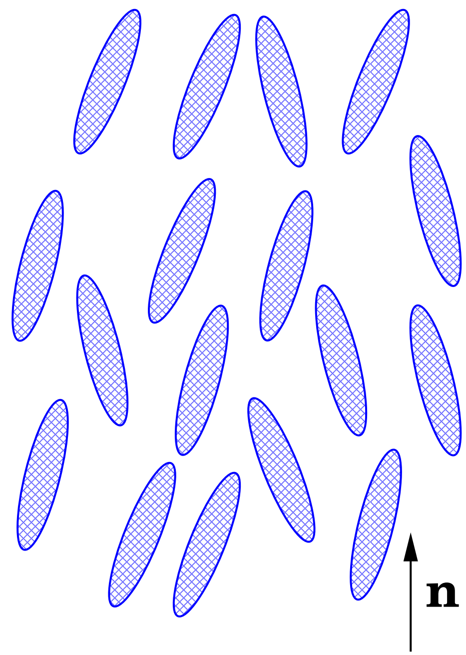


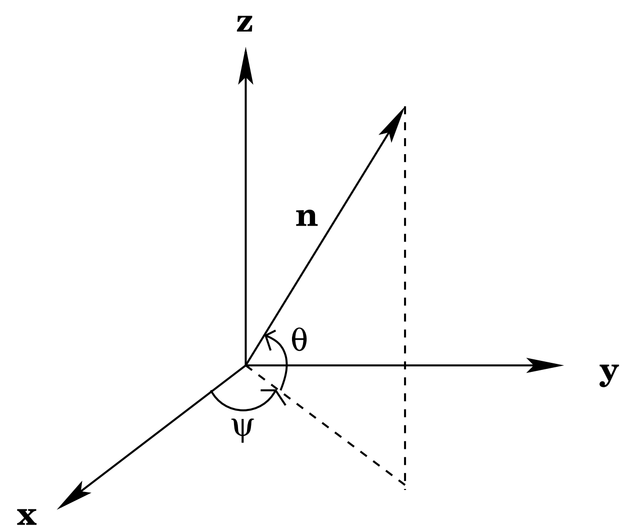
(a) 'off state' $H < H_c$ (b) 'on state' $H > H_c$

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

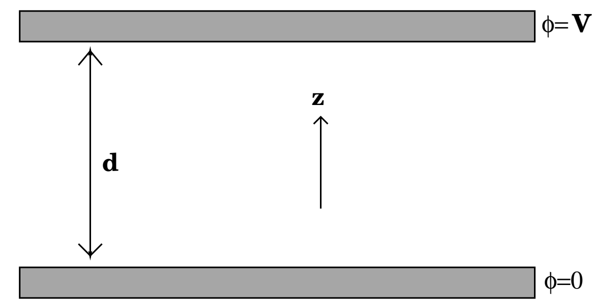
$$\mathcal{F} = \int_V F_{bulk}(\theta, \psi, \nabla\theta, \nabla\psi) + \int_{\mathcal{S}} F_{surface}(\theta, \phi)\, d\mathcal{S}$$

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

- 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

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 $z \in [0, d]$

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

- dielectric anisotropy $\epsilon_a = \epsilon_\| - \epsilon_\perp$, permittivity of free space ϵ_0
- permittivity of free space ϵ_0
- director $\mathbf{n} = (u, v, w)$, $|\mathbf{n}| = 1$
- constraint applied via Lagrange multipliers λ
- electric potential ϕ: $E = \frac{d\phi}{dz}$
- unknowns u, v, w, ϕ, λ

Alternative Model: $\mathcal{Q}$-tensor Theory

- tensor order parameter

$$\mathcal{Q} = \sqrt{\tfrac{3}{2}} S \left(\mathbf{n} \otimes \mathbf{n} - \tfrac{1}{3} I \right)$$

- symmetric tensor

$$\mathcal{Q} = \begin{bmatrix} q_1 & q_2 & q_3 \\ q_2 & q_4 & q_5 \\ q_3 & q_5 & -q_1 - q_4 \end{bmatrix}$$

$$tr(\mathcal{Q}) = 0, \qquad tr(\mathcal{Q}^2) = S^2$$

- five unknowns $\quad q_1, q_2, q_3, q_4, q_5$

Equilibrium Equations 2

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

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

- dimensionless parameters

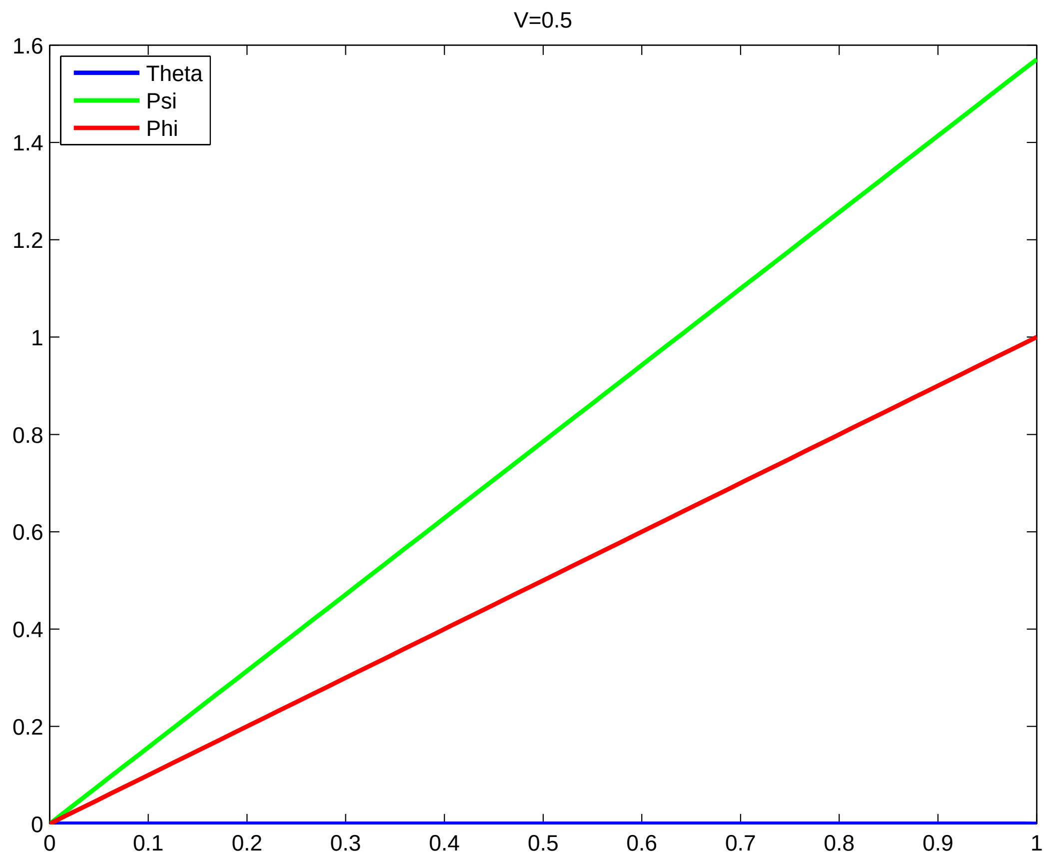
$$\alpha^2 = \frac{\epsilon_0\epsilon_a V^2}{K\pi^2}, \qquad \beta = \frac{\epsilon_\perp}{\epsilon_a}$$

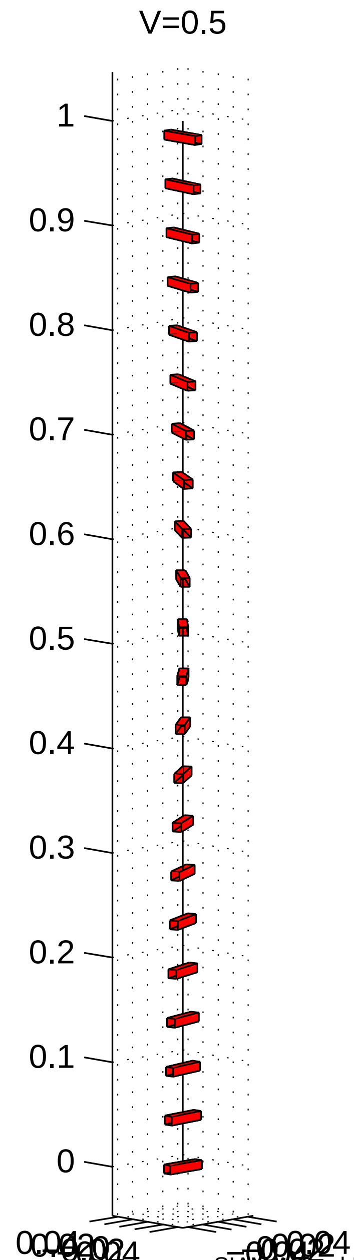
- boundary conditions:

at $z=0$: $\mathbf{n} = (1,0,0)$, at $z=1$: $\mathbf{n} = (0,1,0)$

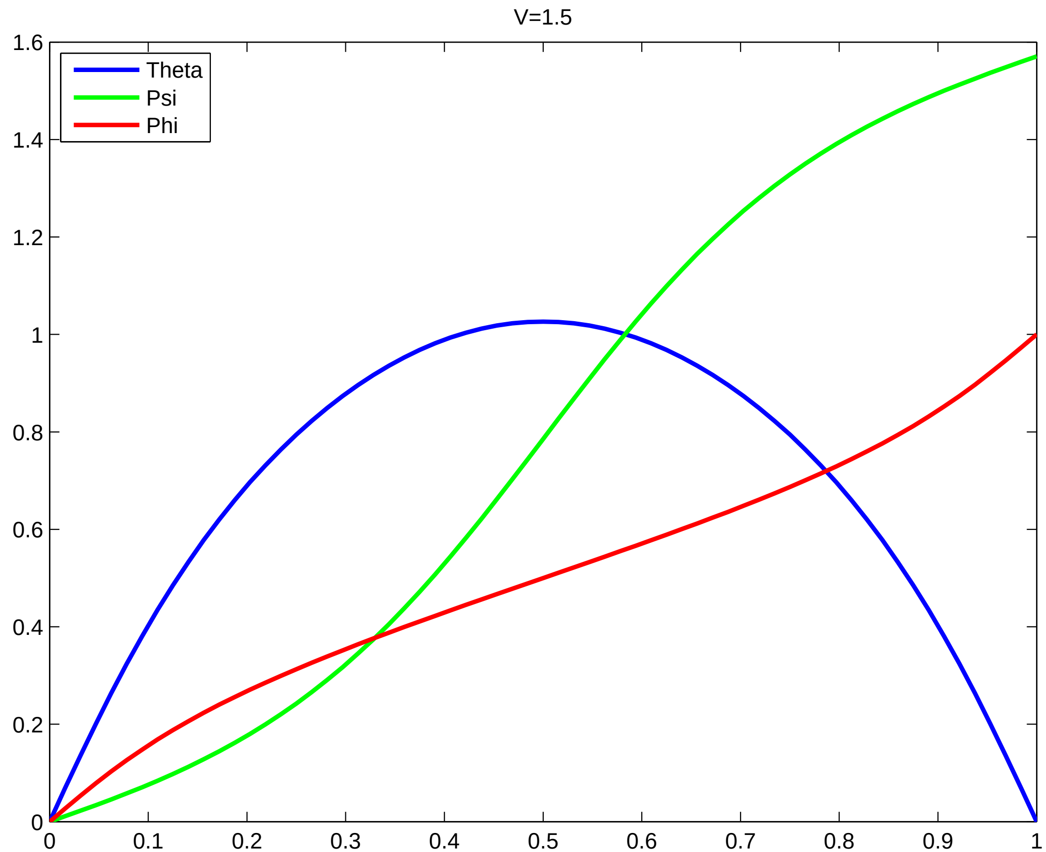
Off State

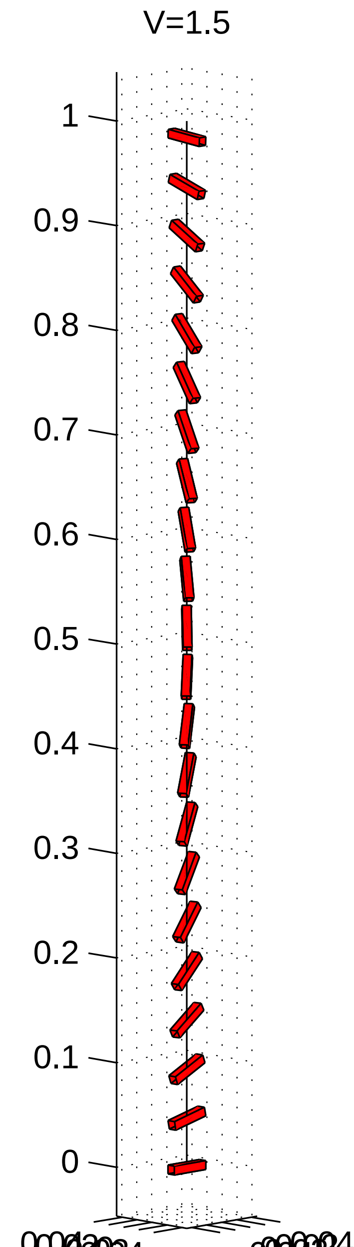
$$\theta(z) \equiv 0, \qquad \psi(z) = \frac{\pi}{2} z, \qquad \phi(z) = z$$





On State


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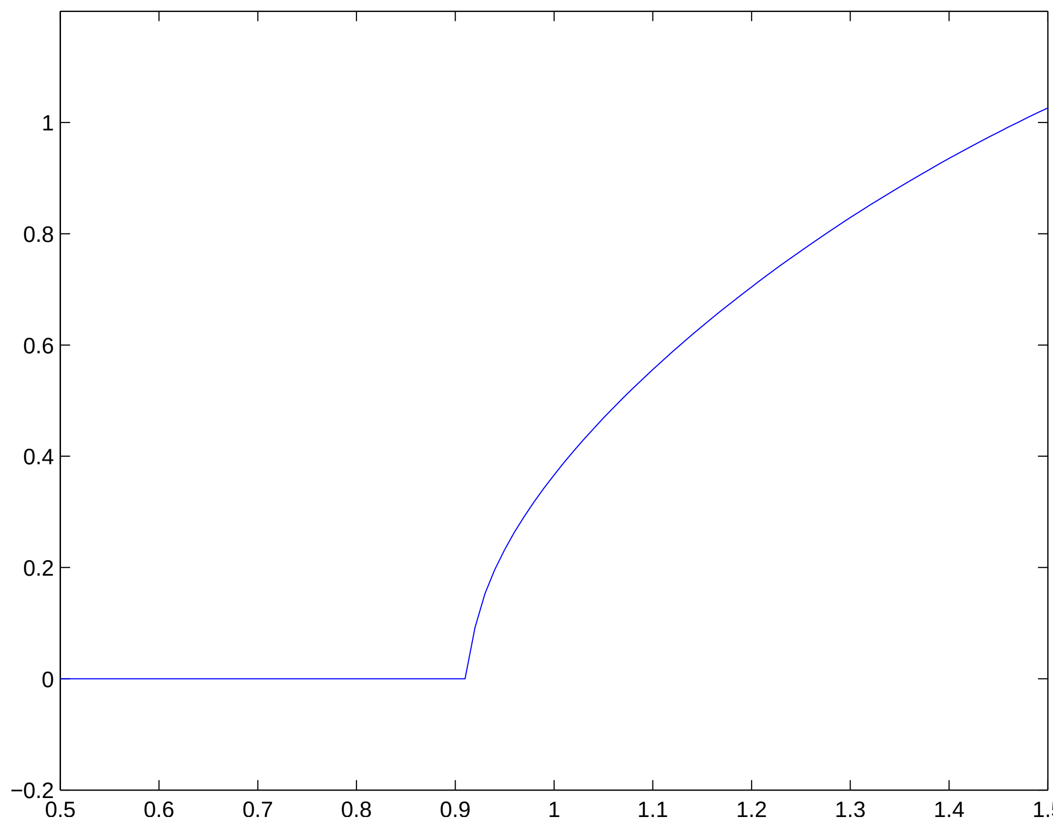
0.3
0.2
0.1
0

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

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- 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

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

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

- $5n \times 5n$ 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: $\nabla^2_{\mathbf{nn}}\mathbf{F} = A$

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

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

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

Eigenvalues of A

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- $\sigma_{\min}(A_{uu}) = \sigma_{\min}(A_{vv}) \simeq \Delta z(\pi^2 - \lambda_1) > 0$

  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 $V < \frac{2}{\sqrt{3}} V_c$

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  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

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

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

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

- information available about basis for nullspace of B^T

Hessian Components 3

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- $C = \frac{1}{\Delta z}\texttt{tri}(-a_{j-\frac{1}{2}}, a_{j-\frac{1}{2}} + a_{j+\frac{1}{2}}, -a_{j+\frac{1}{2}})$

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

$$a_{j+\frac{1}{2}} = \alpha^2\pi^2(\beta + \frac{1}{2}(w^2_j + w^2_{j+1})) > 0$$

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

- diagonally dominant with positive real diagonal entries

C is positive definite

Hessian Components 4

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

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

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

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

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

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- D_w has complex eigenvalues (including one zero)
- $\mathrm{rank}(D) = n - 1$

Full Hessian Structure

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

$$\nabla^2 \mathbf{F} = \begin{bmatrix} A & D & B \\ D^T & -C & 0 \\ B^T & 0 & 0 \end{bmatrix}$$

saddle-point problem

Four Saddle-Point Problems

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

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

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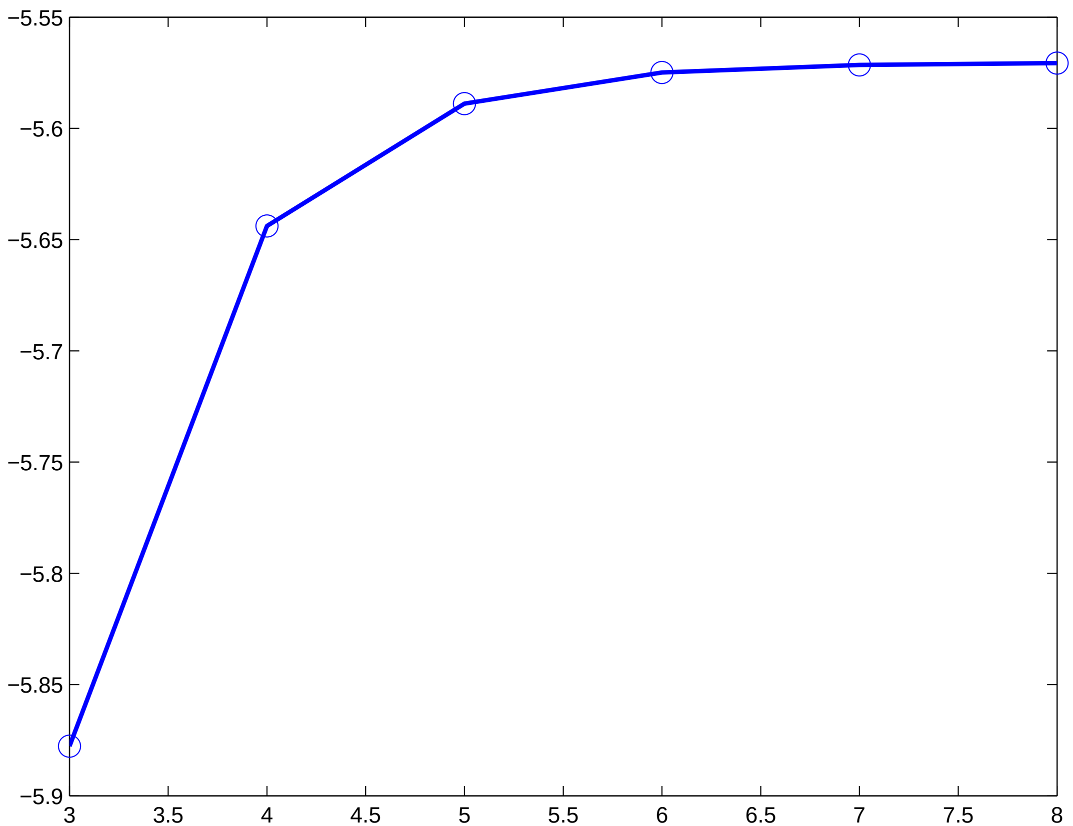
double saddle-point structure

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

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

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

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

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

Constraint-type Preconditioning

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

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

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

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- estimated condition of $C_1^{-1}H$ is $O(N^2)$

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

- estimated condition of $C_2^{-1}H$ is $O(N^2)$

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

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

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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

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- all suggestions welcome!