



# A Monte-Carlo investigation of the nematic-isotropic phase transition

Félix Bunel & Hadrien Vergnet

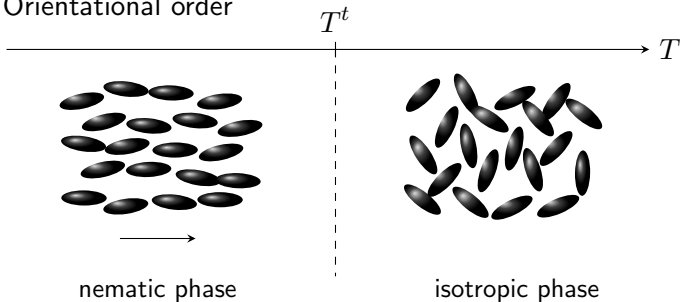
16/01/2017





Nematic phase:

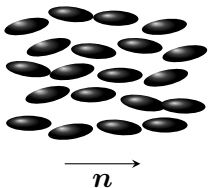
- No positional order
- Orientational order



- 1 The order parameter
- 2 Numerical methods
  - Lebwohl Lasher Model
  - Monte-Carlo Algorithm
  - Equilibration
- 3 Nematic Isotropic Phase Transitions
  - Direct visualisation
  - Energy
  - Order Parameter
  - Histograms
- 4 Influence of an Electric Field
  - Lebwohl Lasher Model
  - Critical point
  - Phase diagram
- 5 Liquid Crystal Display
  - Fréedericksz transition
  - Molecular Orientation

- 1 The order parameter
- 2 Numerical methods
  - Lebwohl Lasher Model
  - Monte-Carlo Algorithm
  - Equilibration
- 3 Nematic Isotropic Phase Transitions
  - Direct visualisation
  - Energy
  - Order Parameter
  - Histograms
- 4 Influence of an Electric Field
  - Lebwohl Lasher Model
  - Critical point
  - Phase diagram
- 5 Liquid Crystal Display
  - Fréedericksz transition
  - Molecular Orientation

# The Order Parameter



$$\mathbf{n} = \langle \mathbf{a} \rangle$$

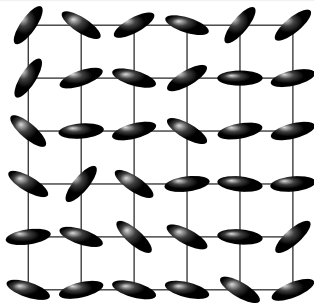


$$S = \frac{3\langle (\mathbf{a} \cdot \mathbf{n})^2 \rangle - 1}{2}$$

Nematic phase :  $S = 1$

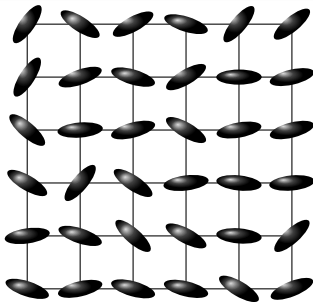
Isotropic phase :  $S = 0$

- 1 The order parameter
- 2 Numerical methods
  - Lebwohl Lasher Model
  - Monte-Carlo Algorithm
  - Equilibration
- 3 Nematic Isotropic Phase Transitions
  - Direct visualisation
  - Energy
  - Order Parameter
  - Histograms
- 4 Influence of an Electric Field
  - Lebwohl Lasher Model
  - Critical point
  - Phase diagram
- 5 Liquid Crystal Display
  - Fréedericksz transition
  - Molecular Orientation

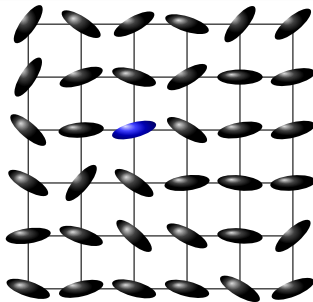


Size :  $30 \times 30 \times 30$

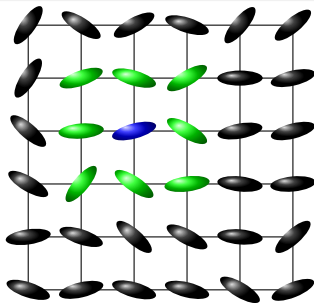
$$E = -\epsilon \sum_{\langle i,j \rangle} \frac{3 \cos^2 \alpha_{i,j} - 1}{2}$$



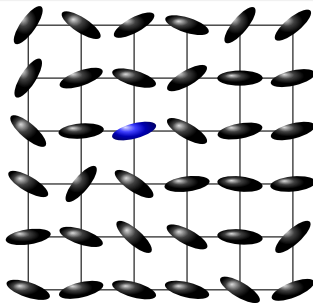




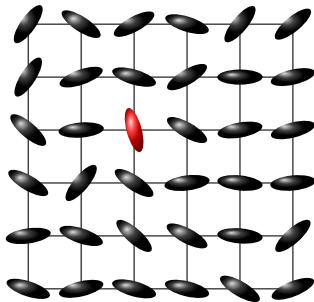
- We select a random site



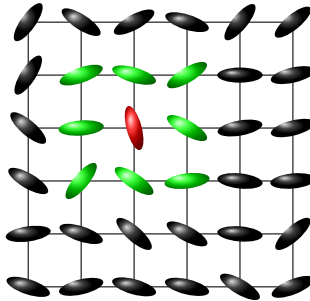
- We select a random site
- We compute the energy with the neighbors :  $E_{old}$



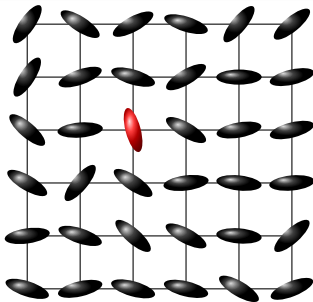
- We select a random site
- We compute the energy with the neighbors :  $E_{old}$
- We try to rotate the chosen site



- We select a random site
- We compute the energy with the neighbors :  $E_{old}$
- We try to rotate the chosen site



- We select a random site
- We compute the energy with the neighbors :  $E_{old}$
- We try to swap the chosen site
- We compute the energy with the neighbors :  $E_{new}$

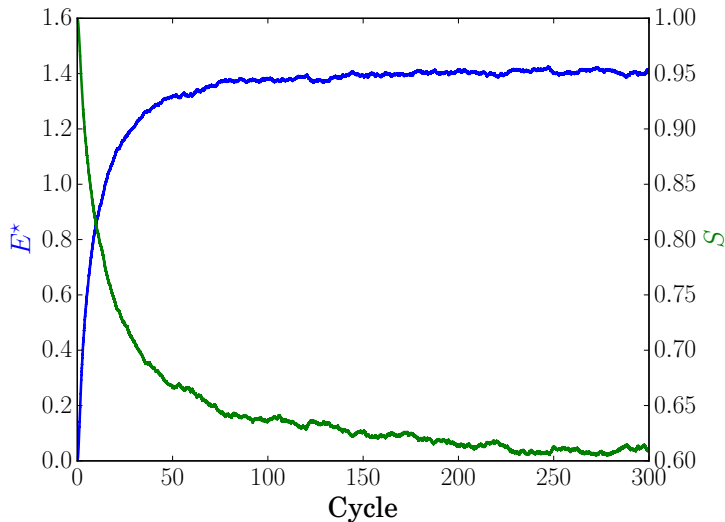


- We select a random site
- We compute the energy with the neighbors :  $E_{old}$
- We try to swap the chosen site
- We compute the energy with the neighbors :  $E_{new}$
- We accept the swap with a probability :

$$p = e^{-\frac{E_{old} - E_{new}}{k_B T}}$$

# Numerical Methods

## Equilibration



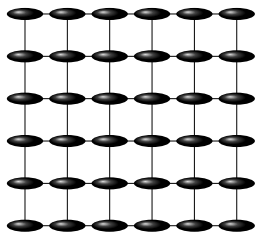
Equilibration at  $T^* = 1$

- 1 The order parameter
- 2 Numerical methods
  - Lebwohl Lasher Model
  - Monte-Carlo Algorithm
  - Equilibration
- 3 Nematic Isotropic Phase Transitions
  - Direct visualisation
  - Energy
  - Order Parameter
  - Histograms
- 4 Influence of an Electric Field
  - Lebwohl Lasher Model
  - Critical point
  - Phase diagram
- 5 Liquid Crystal Display
  - Fréedericksz transition
  - Molecular Orientation

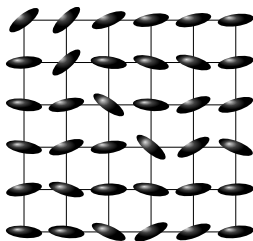


# Nematic Isotropic Phase Transitions

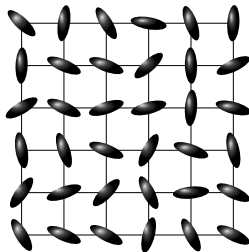
Direct visualisation



$$T^* = 0.05$$



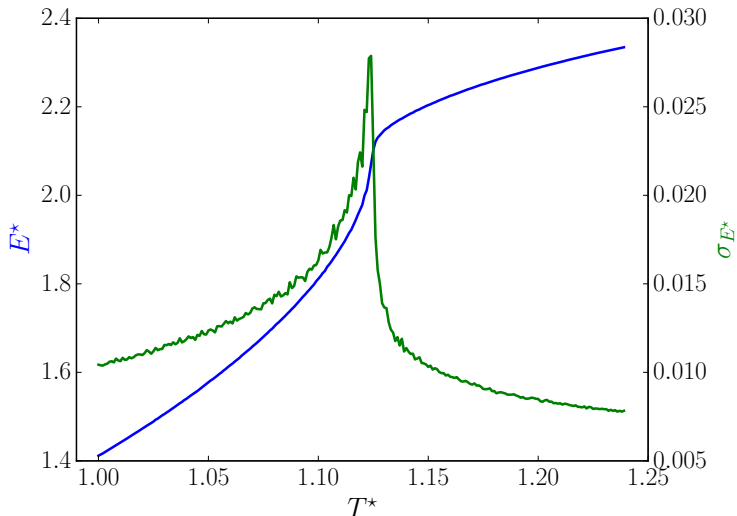
$$T^* = 0.9$$



$$T^* = 1.5$$

# Nematic Isotropic Phase Transitions

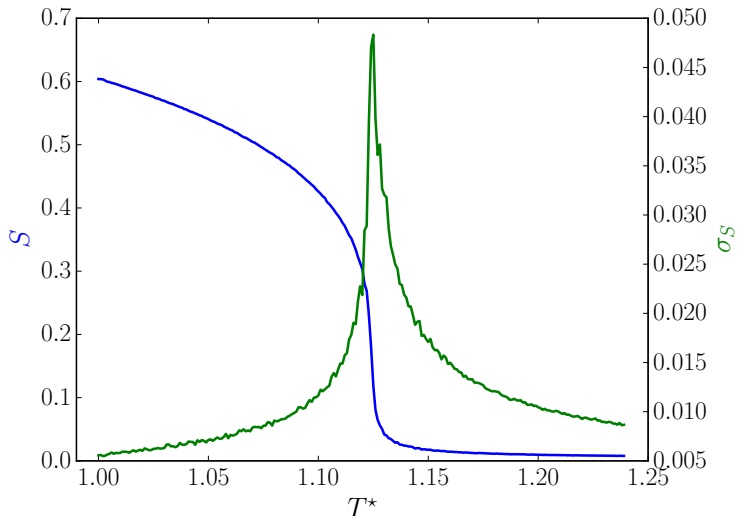
Energy



Energy and its variance.

# Nematic Isotropic Phase Transitions

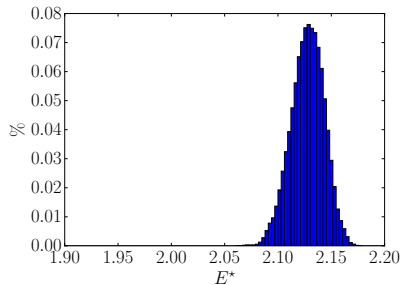
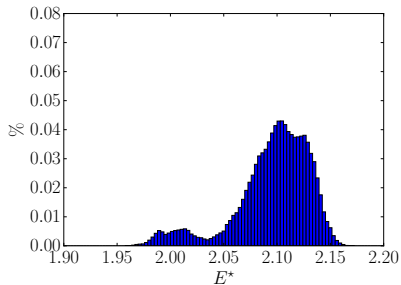
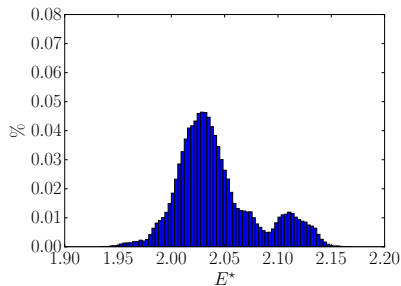
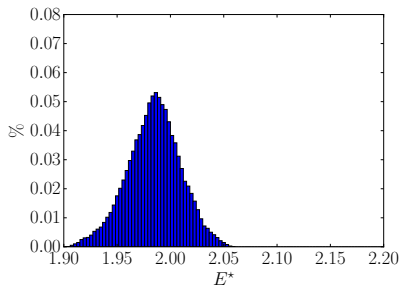
Order Parameter



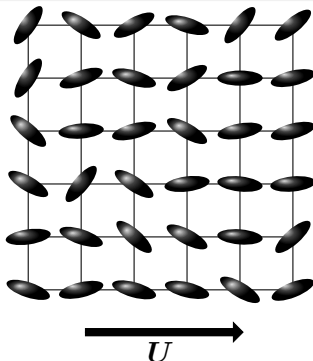
Order parameter and its variance.

# Nematic Isotropic Phase Transitions

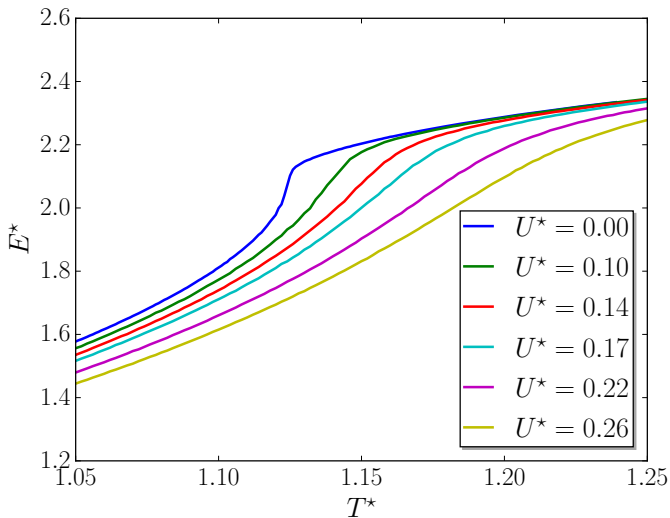
## Energy Histograms



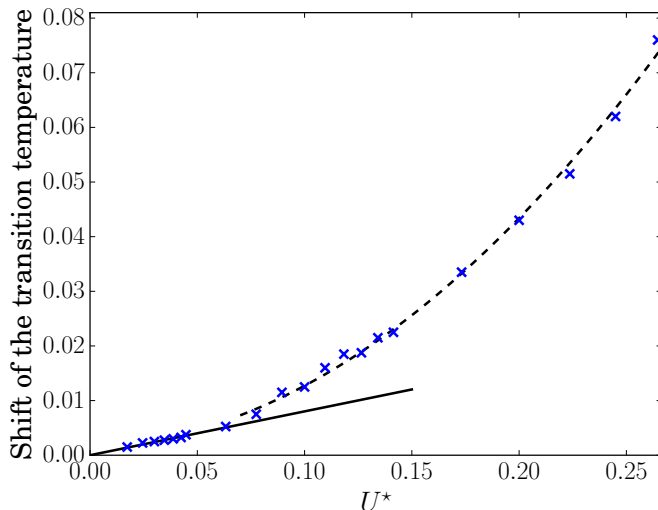
- 1 The order parameter
- 2 Numerical methods
  - Lebwohl Lasher Model
  - Monte-Carlo Algorithm
  - Equilibration
- 3 Nematic Isotropic Phase Transitions
  - Direct visualisation
  - Energy
  - Order Parameter
  - Histograms
- 4 Influence of an Electric Field
  - Lebwohl Lasher Model
  - Critical point
  - Phase diagram
- 5 Liquid Crystal Display
  - Fréedericksz transition
  - Molecular Orientation



$$E = -\epsilon \sum_{\langle i,j \rangle} \frac{3 \cos^2 \alpha_{i,j} - 1}{2} - \epsilon \xi U^2 \sum_i \frac{3 \cos^2 \beta_i - 1}{2}$$



Energy for different electric fields.



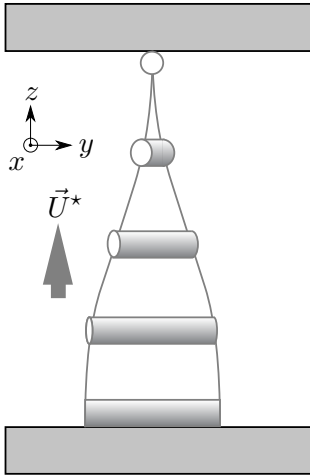
Transition temperature as a function of the electric field.



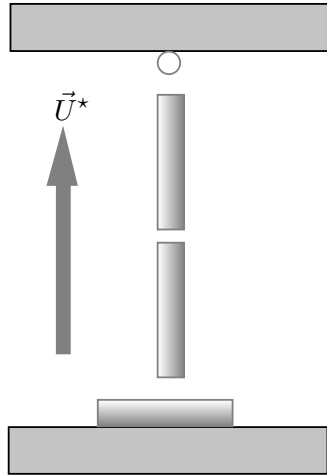
- 1 The order parameter
- 2 Numerical methods
  - Lebwohl Lasher Model
  - Monte-Carlo Algorithm
  - Equilibration
- 3 Nematic Isotropic Phase Transitions
  - Direct visualisation
  - Energy
  - Order Parameter
  - Histograms
- 4 Influence of an Electric Field
  - Lebwohl Lasher Model
  - Critical point
  - Phase diagram
- 5 Liquid Crystal Display
  - Fréedericksz transition
  - Molecular Orientation

# Liquid Crystal Display

## Fréedericksz transition



(a) Pixel "off" state

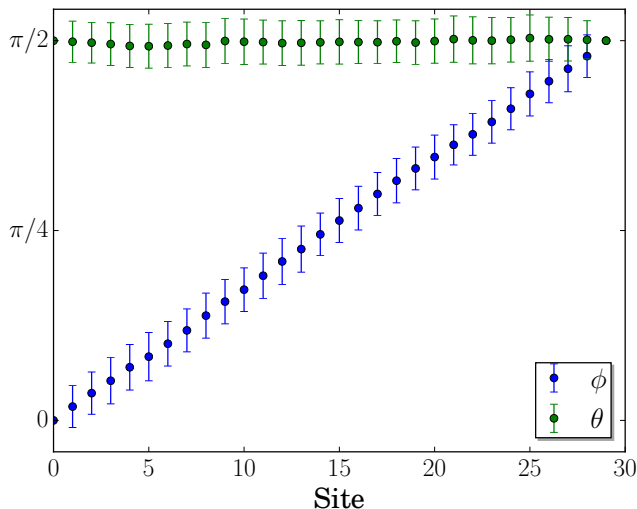


(b) Pixel "on" state

Diagram of a LCD pixel using *twisted nematic* technology.

# Liquid Crystal Display

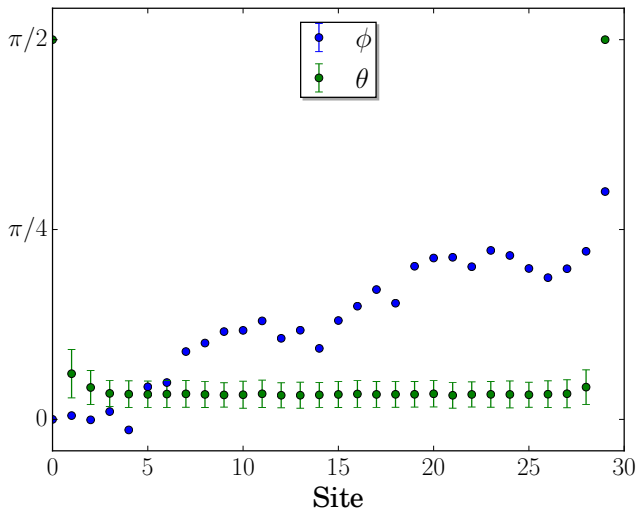
## Molecule Orientation



Molecule orientation **without** electric field

# Liquid Crystal Display

## Molecule Orientation



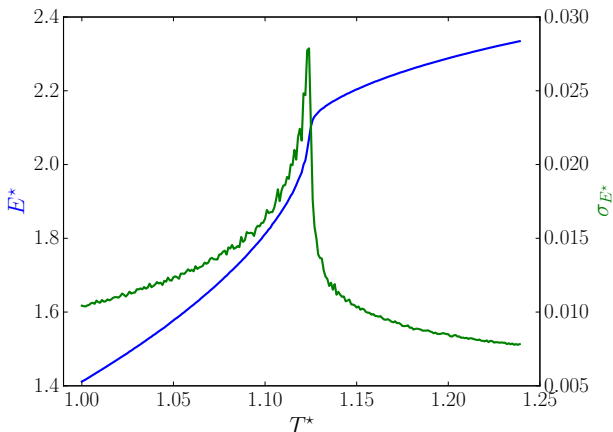
Molecule orientation **with** electric field

# Conclusion

# Conclusion

Detailed study of nematic-isotropic transition with Lebwohl-Laser model :

- first order transition at  $T^* = 1.1232 \pm 0.0005$



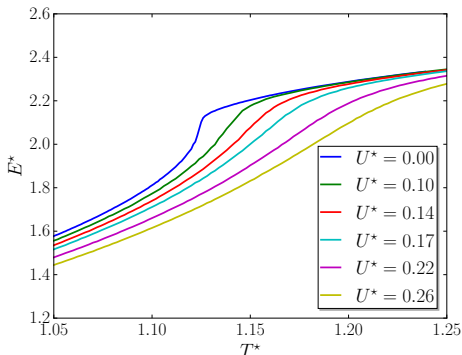
# Conclusion

Detailed study of nematic-isotropic transition with Lebwohl-Laser model :

- first order transition at  $T^* = 1.1232 \pm 0.0005$

Electric field influence :

- shifts transition temperature and critical point for strong fields



# Conclusion

Detailed study of nematic-isotropic transition with Lebwohl-Laser model :

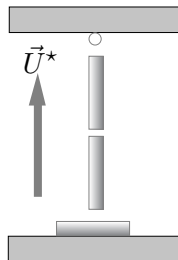
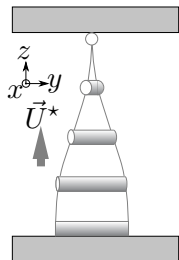
- first order transition at  $T^* = 1.1232 \pm 0.0005$

Electric field influence :

- shifts transition temperature and critical point for strong fields

LCD and Fréedericksz :

- Lebwohl-Laser model can be used to model a LCD pixel





Perspectives :

- Find the value of the critical field in that Fréedericksz transition
- Study the temperature dependence of that transition

Thank you for your attention