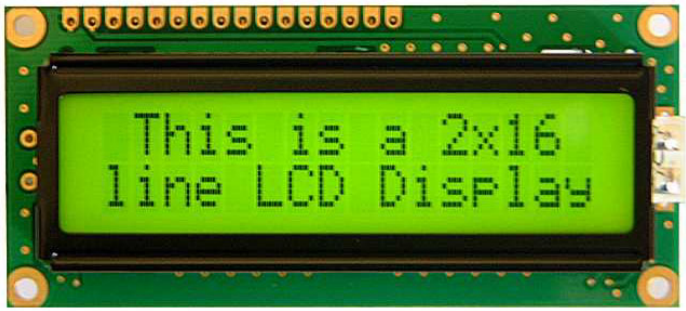
A Monte-Carlo investigation of the nematic-isotropic phase transition

Félix Bunel & Hadrien Vergnet

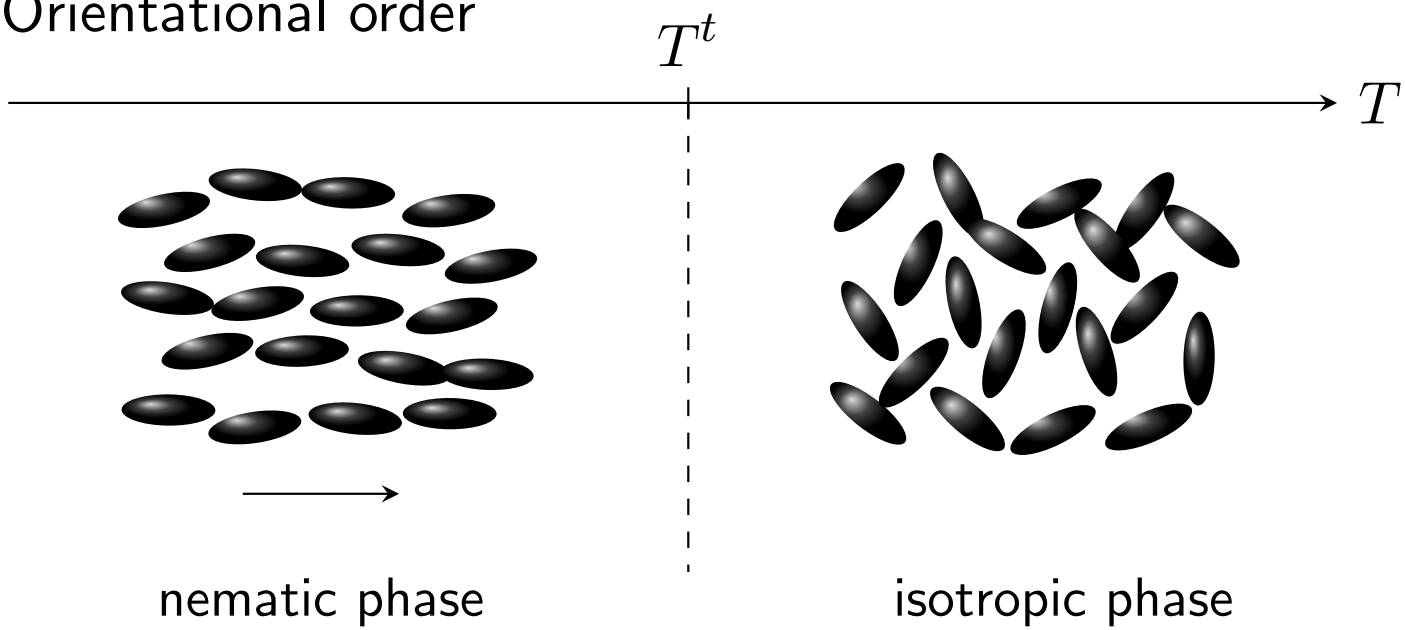
16/01/2017

Introduction



Nematic phase:

- No positional order
- Orientational order



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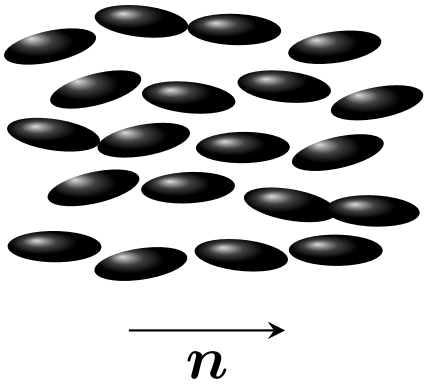
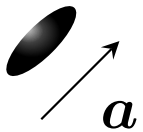
The Order Parameter

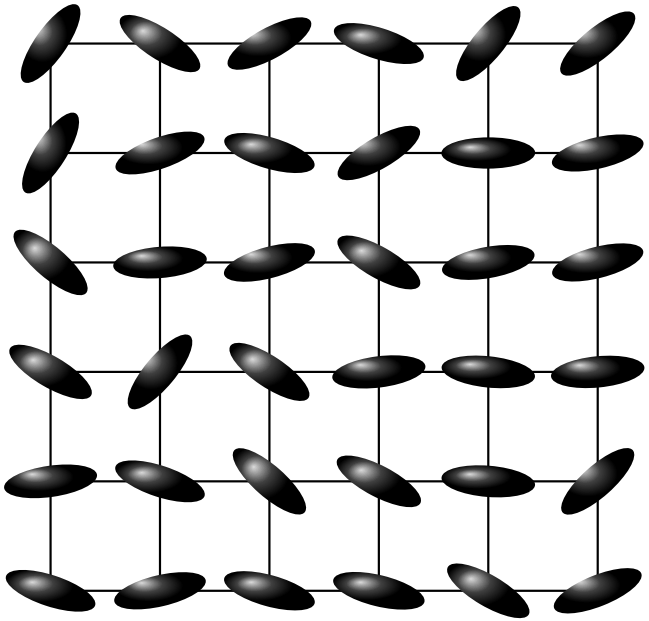


$$\boldsymbol{n} = \langle \boldsymbol{a} \rangle$$



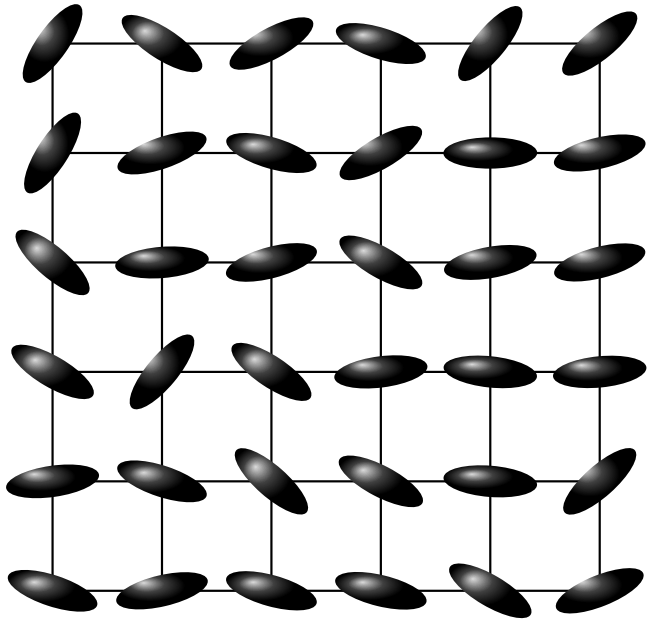
$$S = \frac{3\langle (\boldsymbol{a} \cdot \boldsymbol{n})^2 \rangle - 1}{2}$$

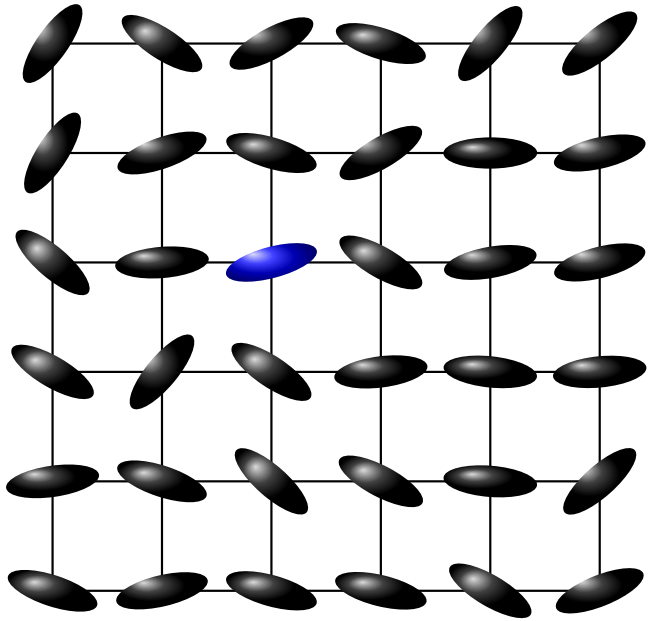
Nematic phase : $S = 1$ Isotropic phase : $S = 0$



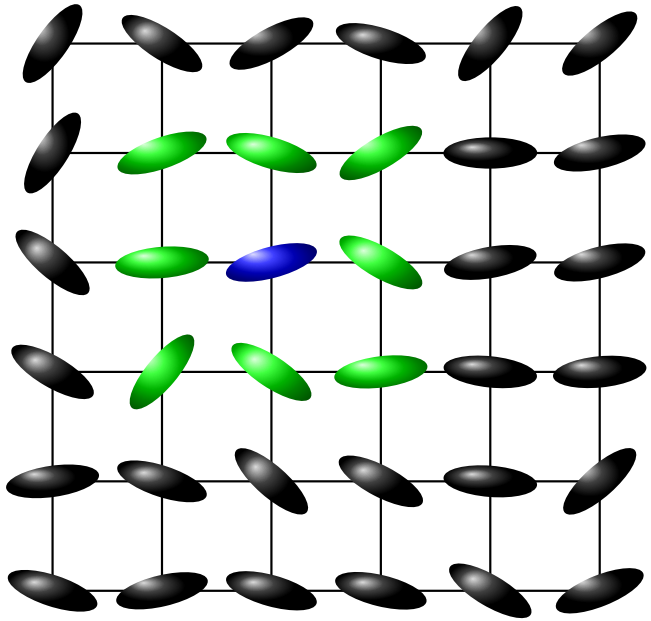
Size : $30 \times 30 \times 30$

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

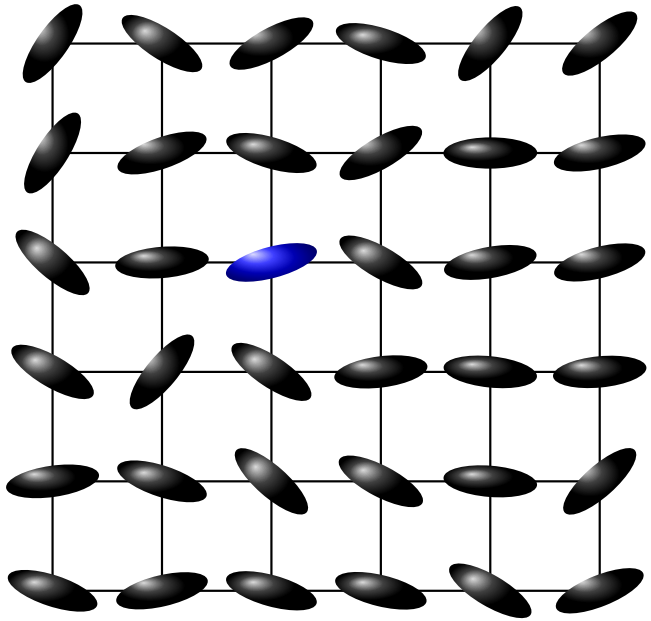




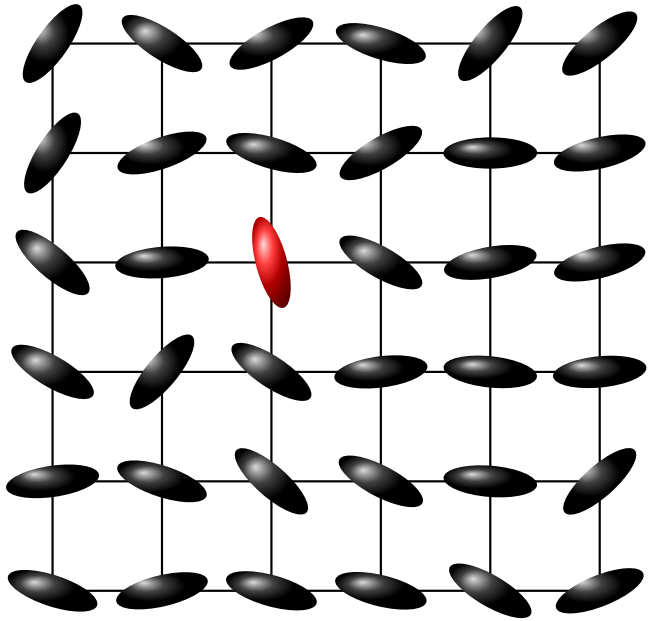
- We select a random site



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



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



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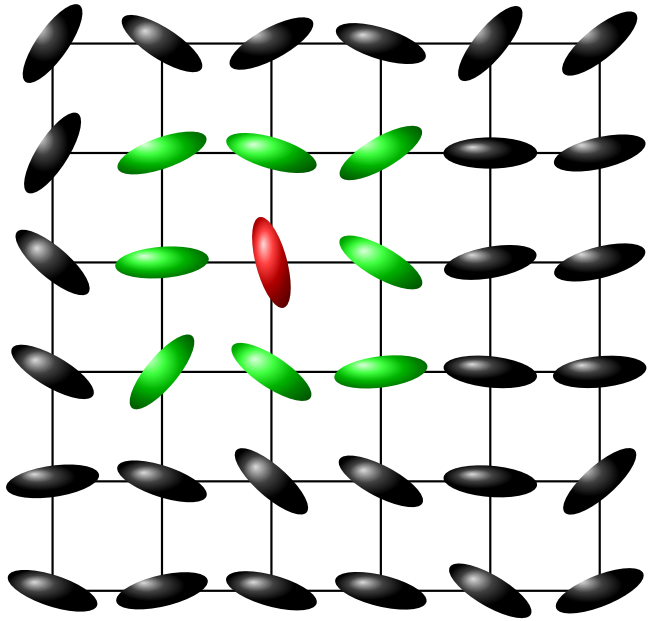
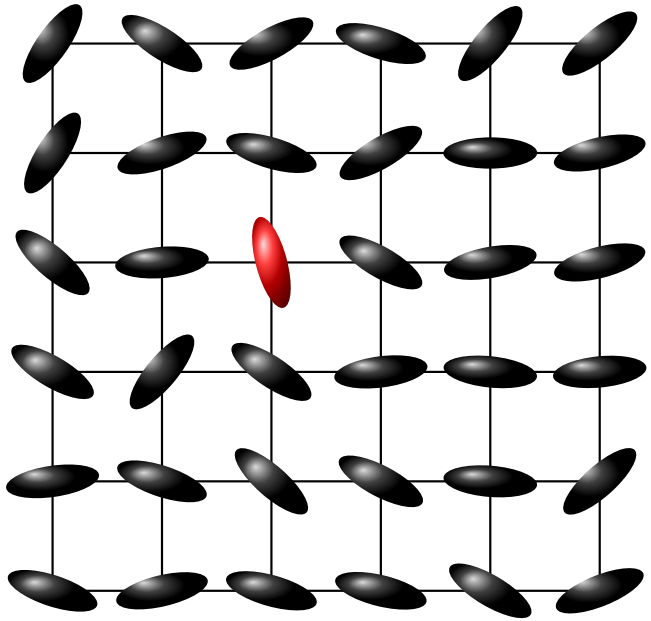
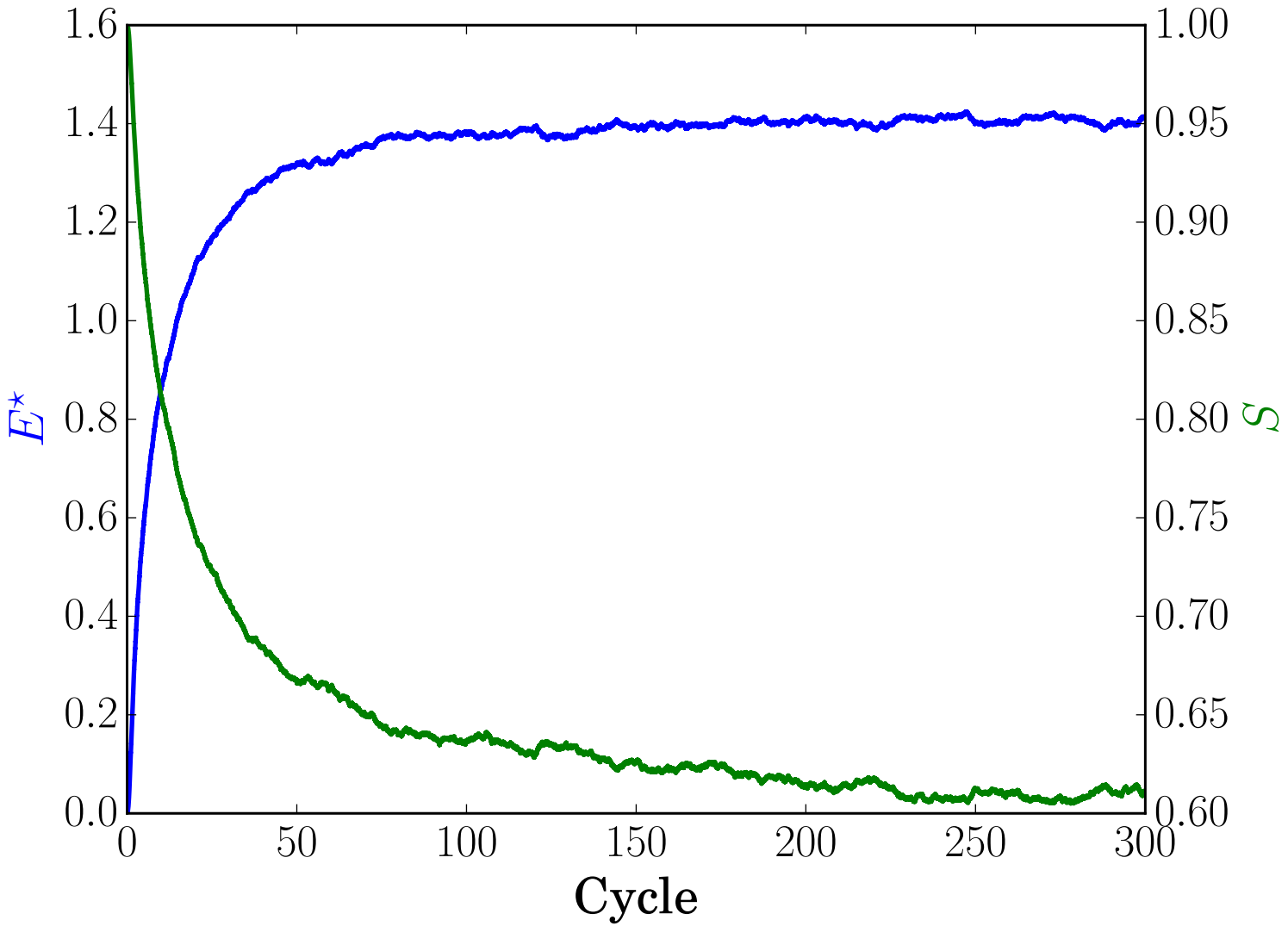


- We select a random site
- We compute the energy with the neighboors : E_{old}
- We try to swap the chosen site
- We compute the energy with the neighboors : E_{new}



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

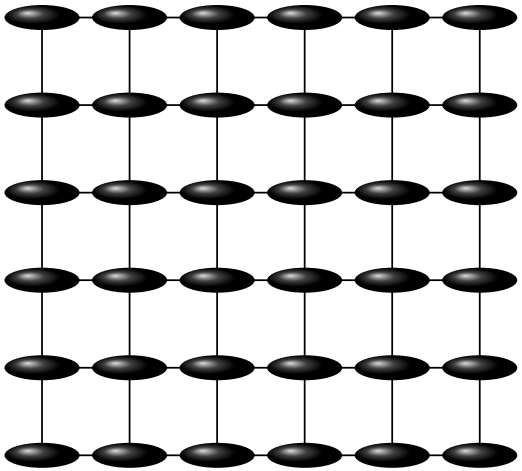
$$p = e^{-\frac{E_{old} - E_{new}}{k_B T}}$$



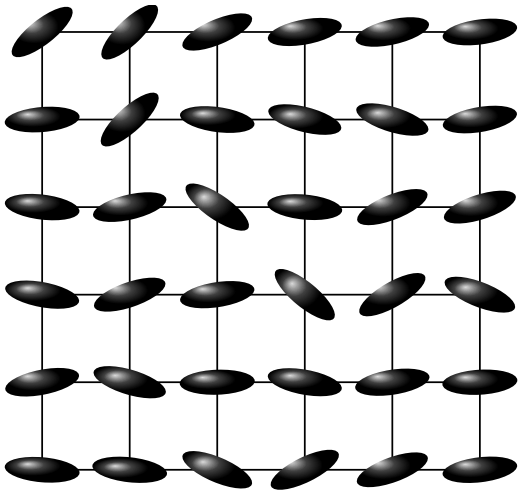
Equilibration at $T^\star = 1$

Nematic Isotropic Phase Transitions

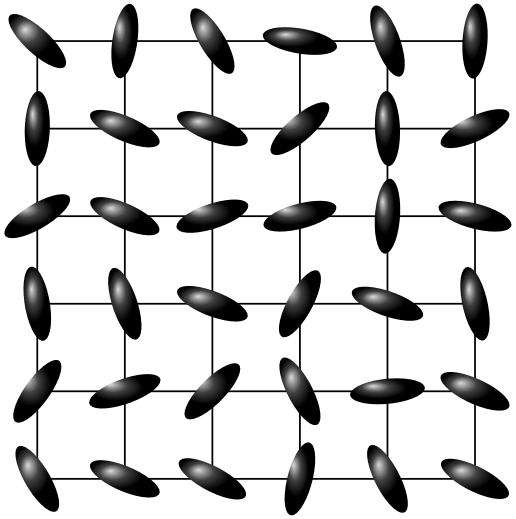
Direct visualisation



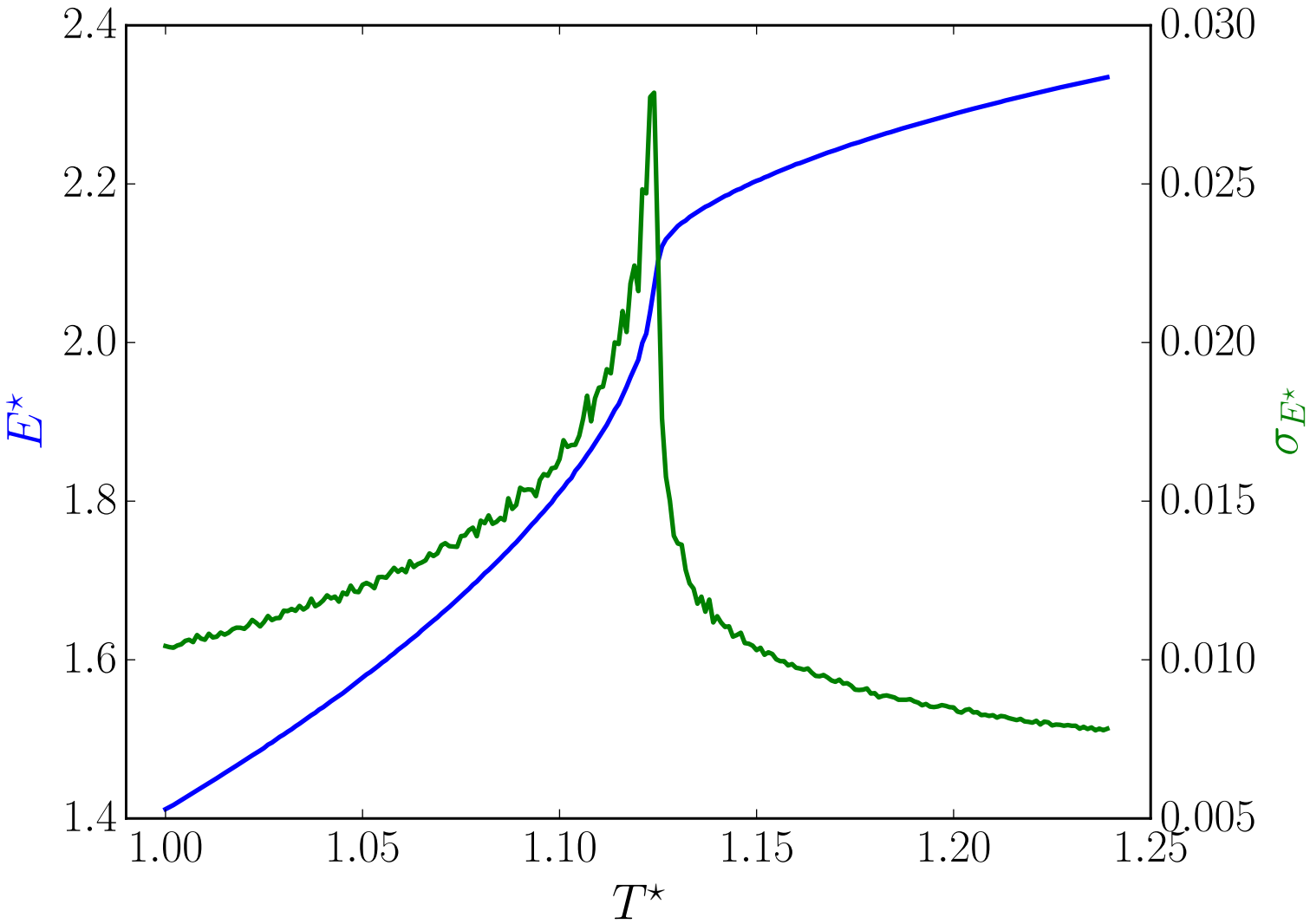
$T^\star = 0.05$



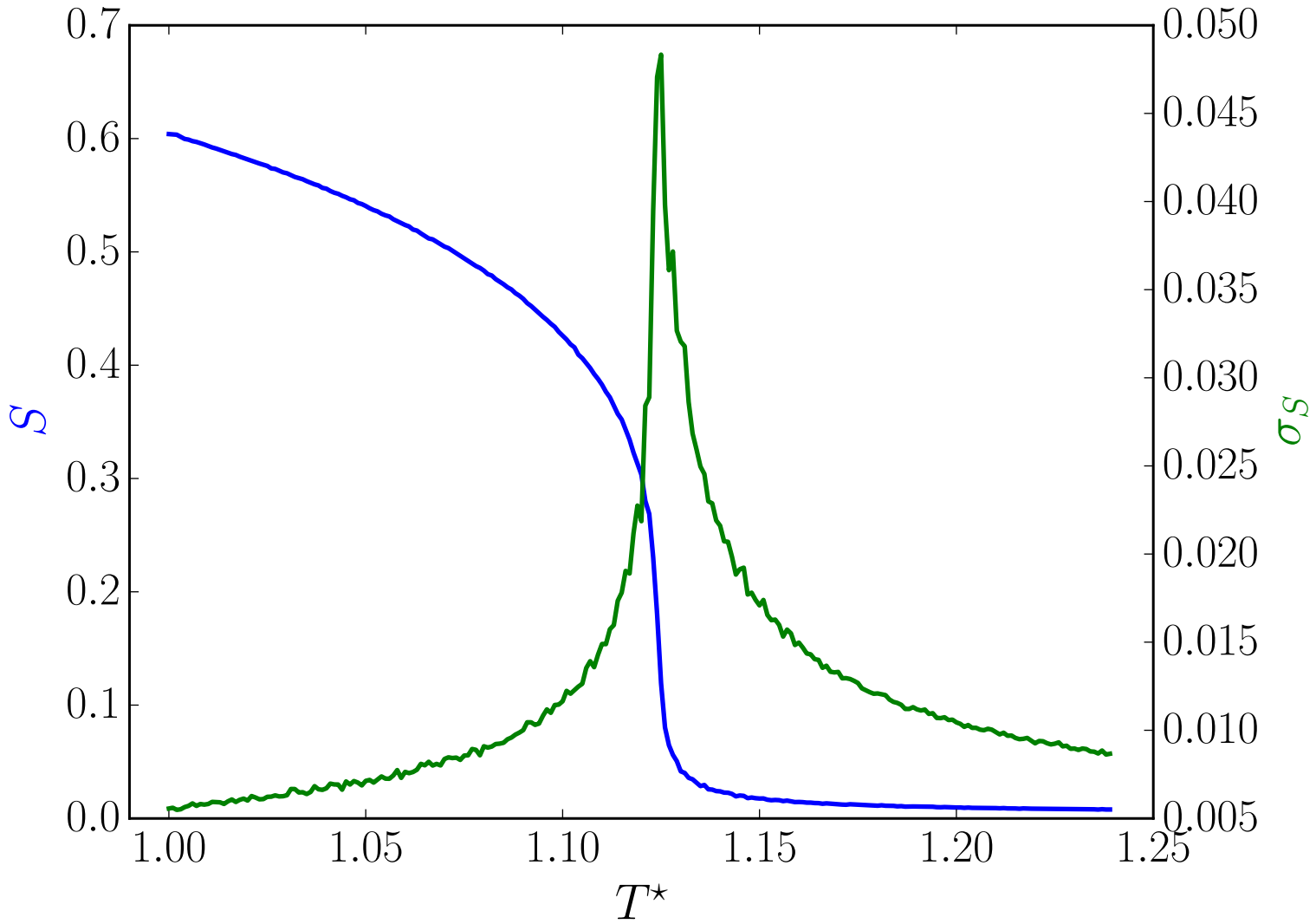
$T^\star = 0.9$



$T^\star = 1.5$



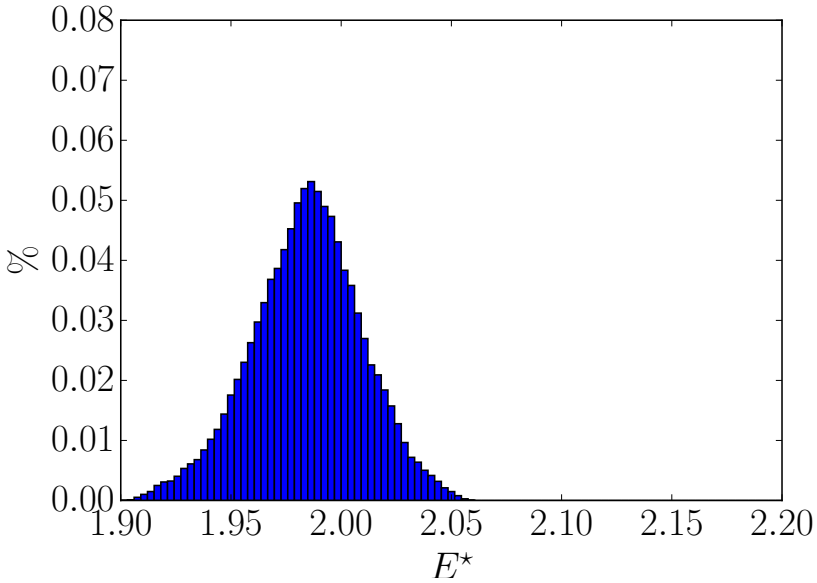
Energy and its variance.

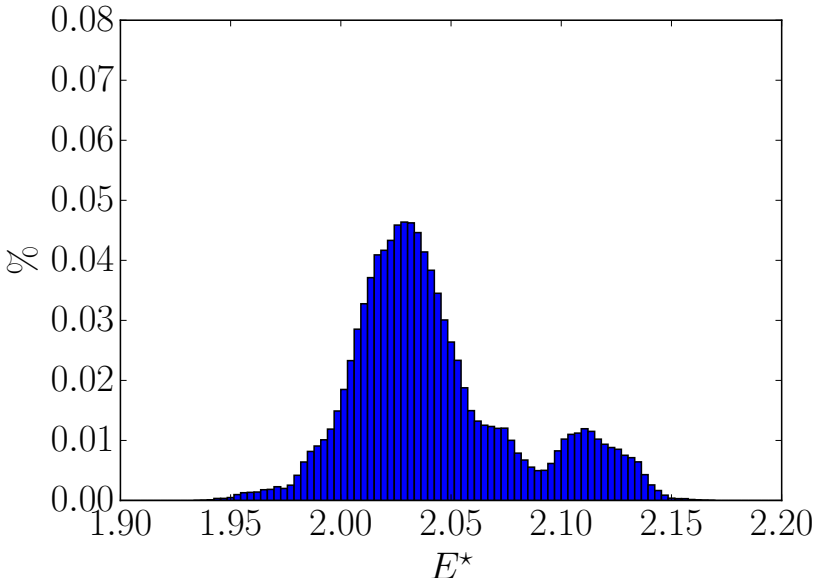


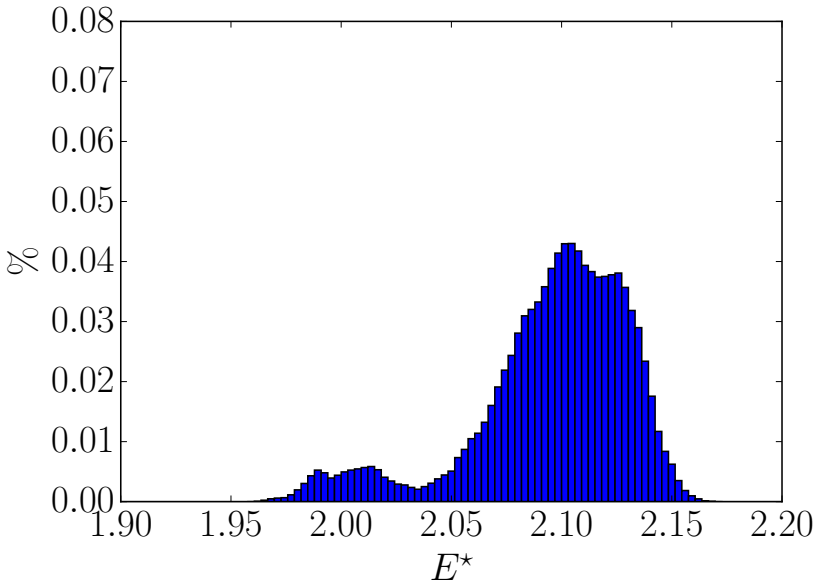
Order parameter and its variance.

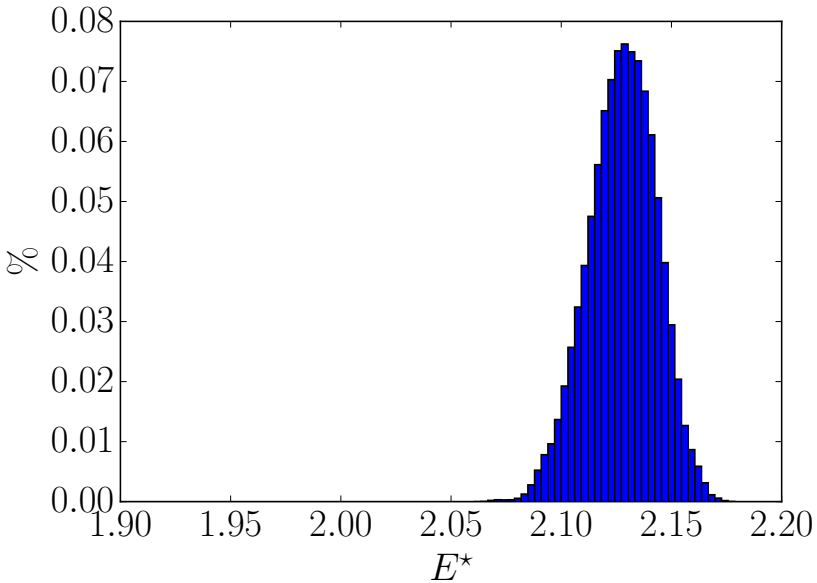
Nematic Isotropic Phase Transitions

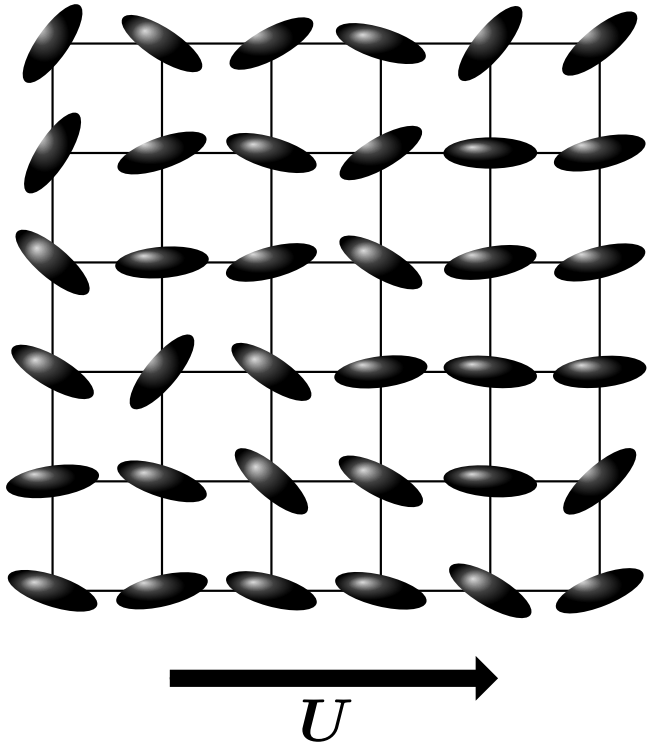
Energy Histograms



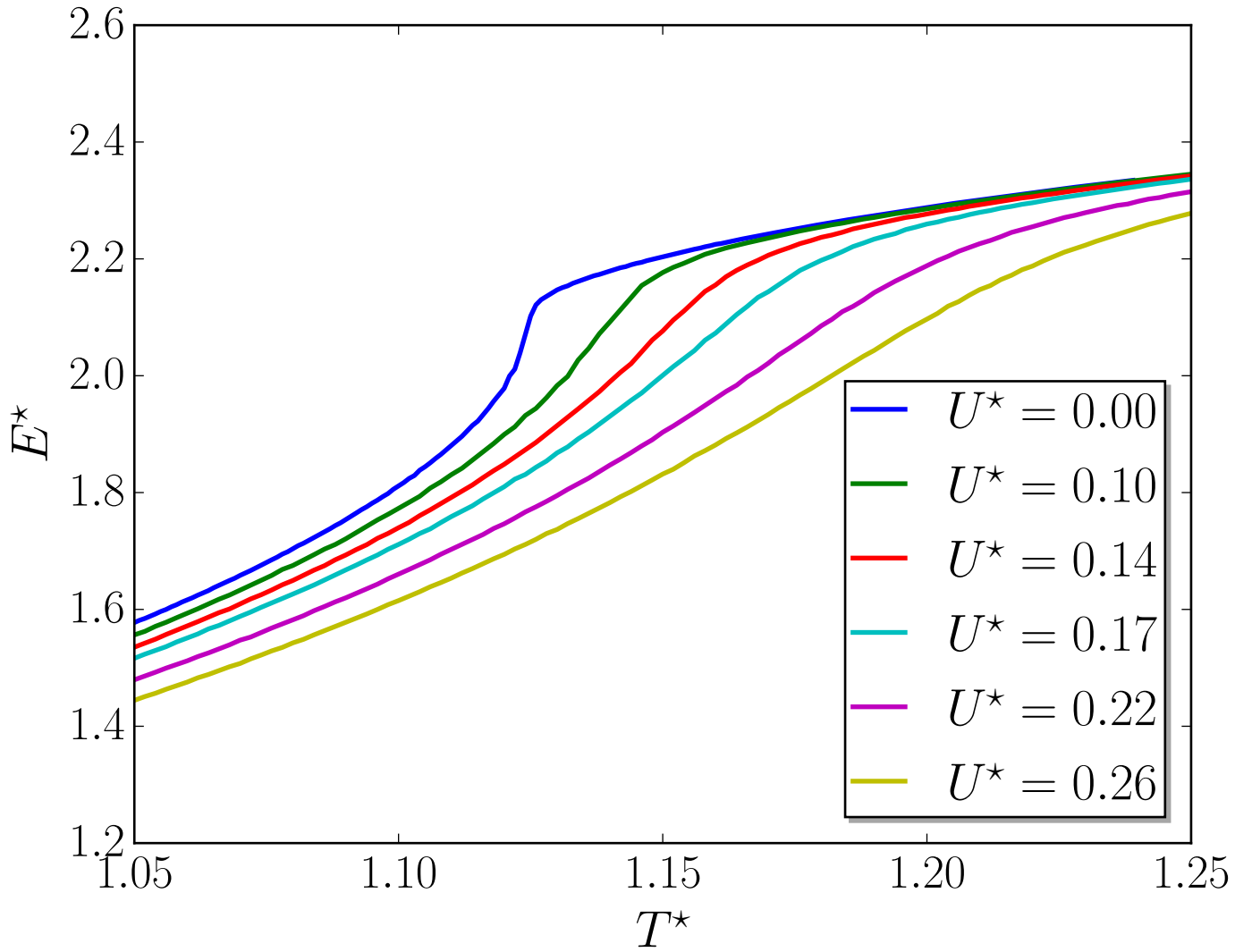




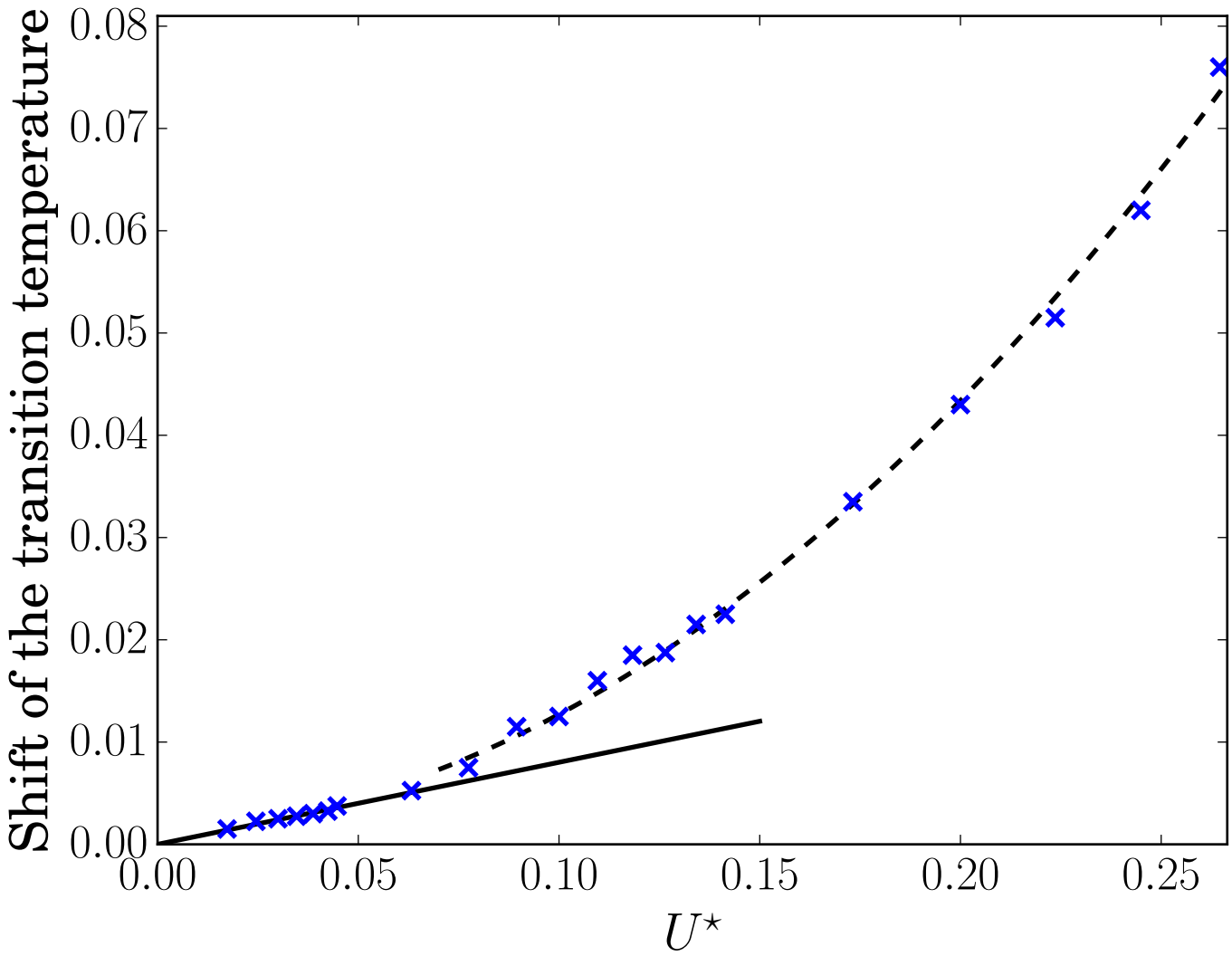




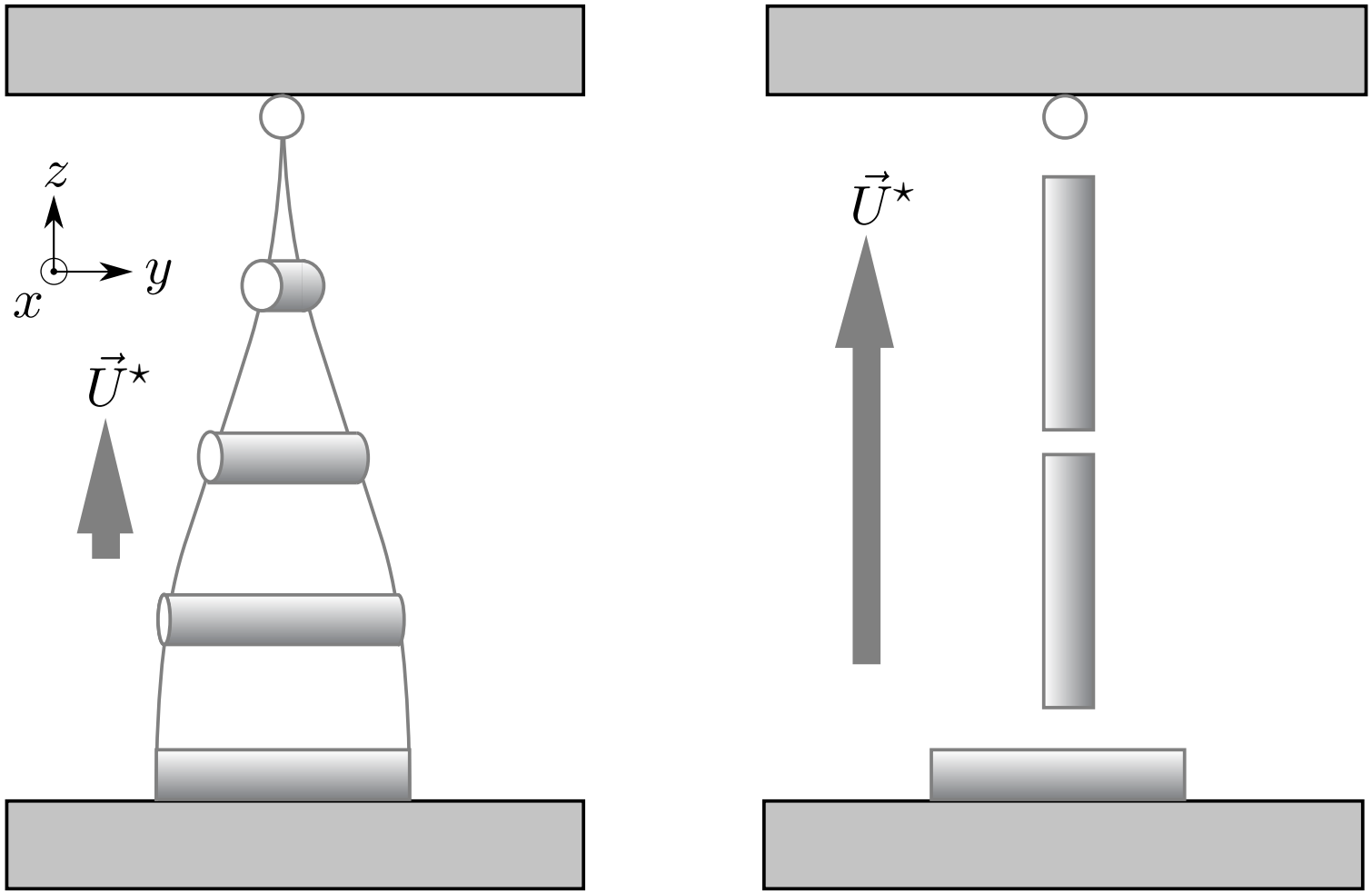
$$E = -\epsilon \sum_{<i,j>} \frac{3\cos^2 \alpha_{i,j} - 1}{2} - \epsilon \xi U^2 \sum_i \frac{3\cos^2 \beta_i - 1}{2}$$



Energy for different electric fields.



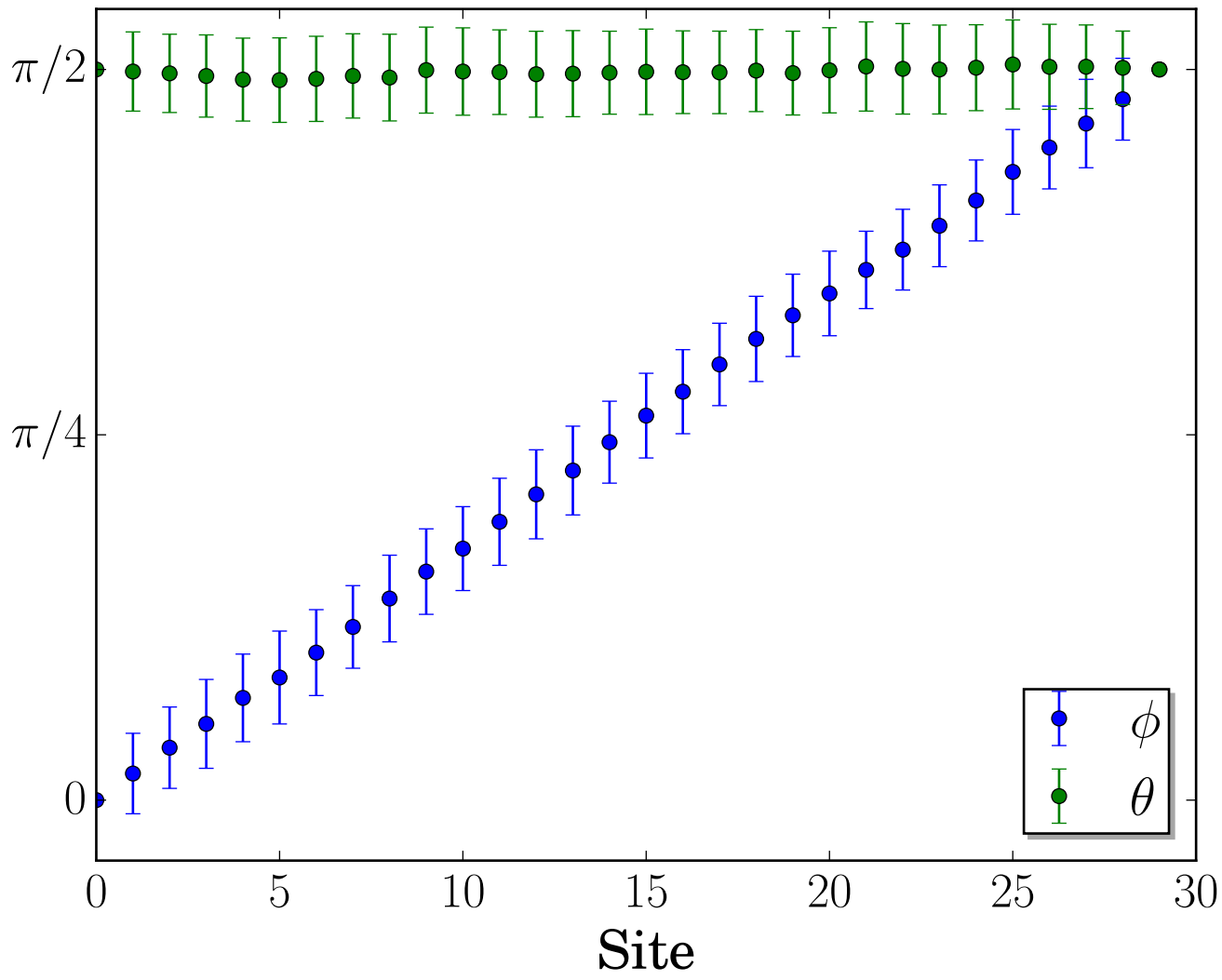
Transition temperature as a function of the electric field.



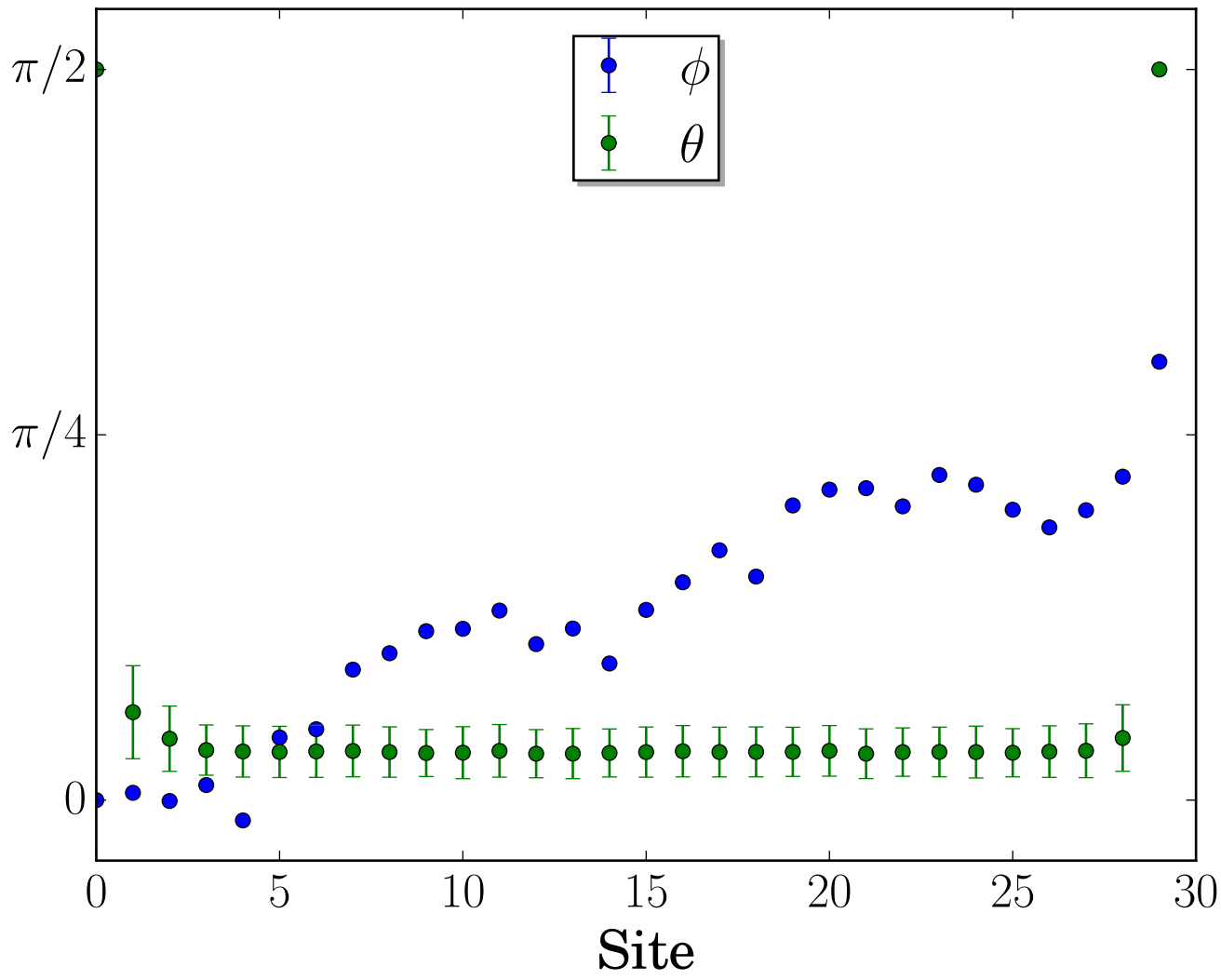
(a) Pixel "off" state

(b) Pixel "on" state

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



Molecule orientation **without** electric field



Molecule orientation **with** electric field

Conclusion

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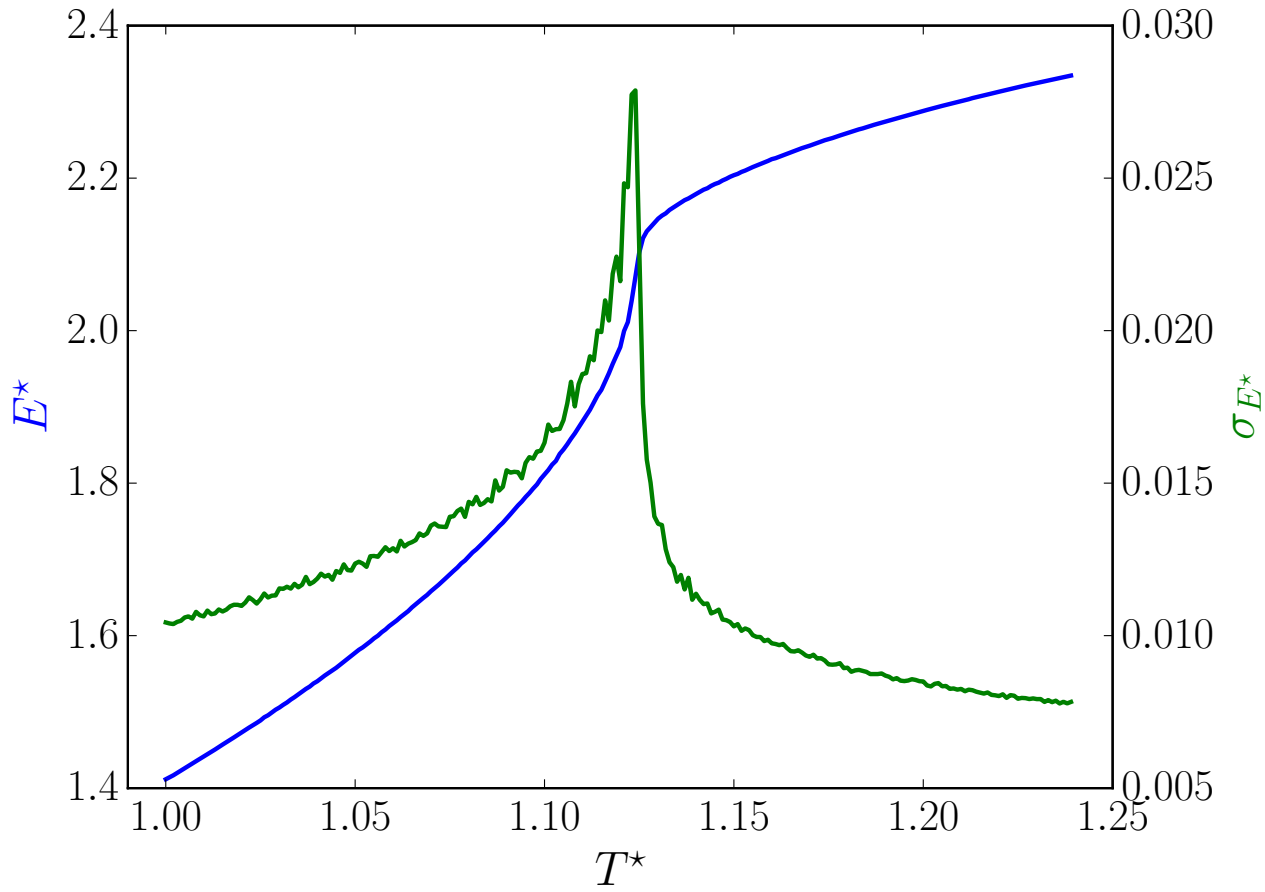
Detailed study of nematic-isotropic transition with Lebwohl-Laser model :

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



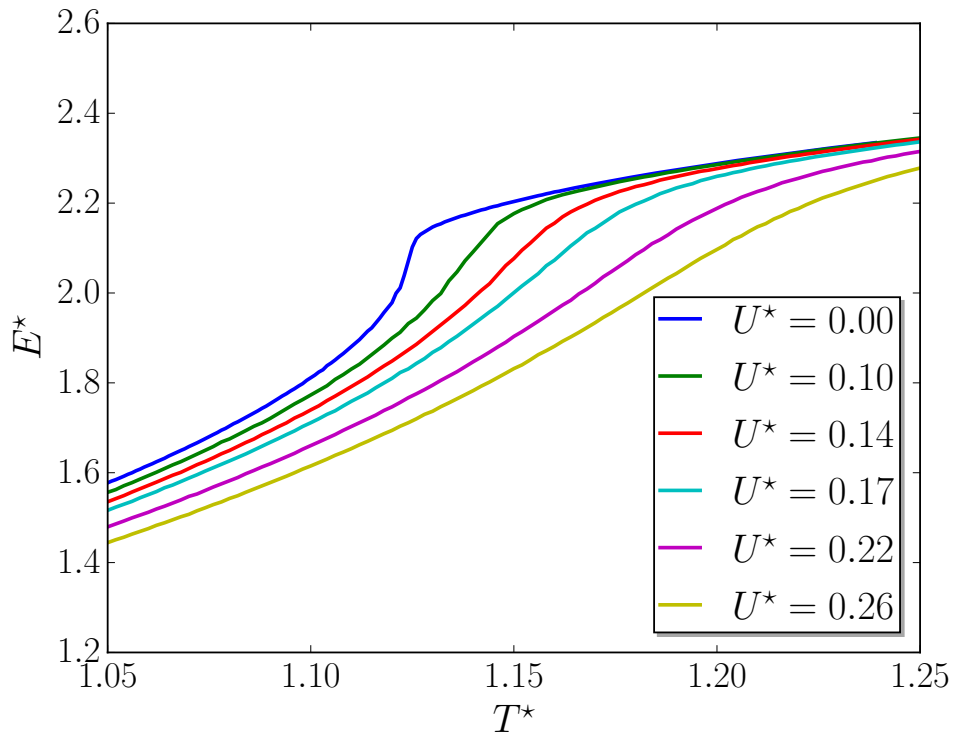
Conclusion

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

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

Electric field influence :

- shifts transition temperature and critical point for strong fields



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

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

Electric field influence :

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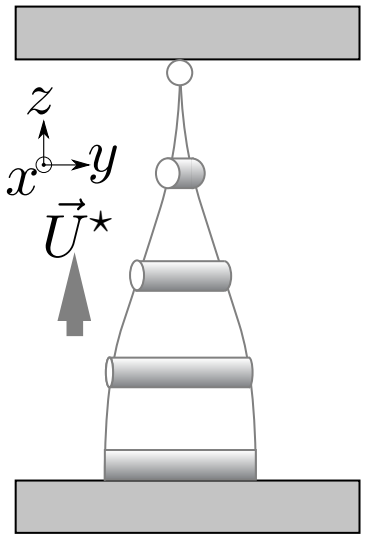
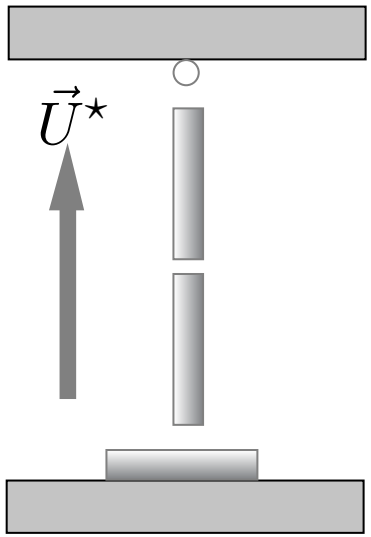
LCD and Fréedericksz :

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





Perspectives

Perspectives :

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

Thank you for your attention