Transfer-matrix method for liquid crystals

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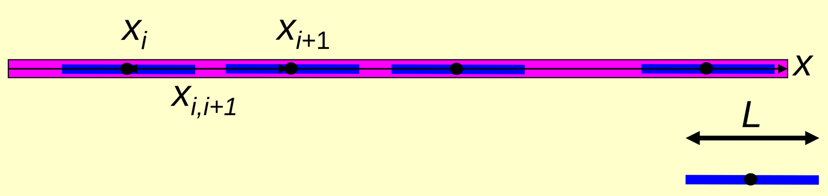
Tonks-gas



Pair potencial: $u(x_{i,i+1}) = \begin{cases} \infty, & x_{i,i+1} \le L \\ 0, & x_{i,i+1} > L \end{cases}$

Isobaric partition function:

$$Q_{NPT} = \frac{1}{\Lambda^N} \int dx_1..dx_N \exp\left(-\beta \sum_{i=1}^{N} \left(u(x_{i,i+1}) + P x_{i,i+1}\right)\right)$$

$x_i \to x_{i,i+1}$

$$Q_{NPT} = \frac{1}{\Lambda^N} \int_L^\infty dx_{1,2} ... \int_L^\infty dx_{N,N+1} \exp(-\beta P x_{1,2}) ... \exp(-\beta P x_{N,N+1})$$

$$Q_{NPT} = \frac{\exp(-\beta P L)^N}{(\beta P)^N \Lambda^N}$$

Gibbs free energy:

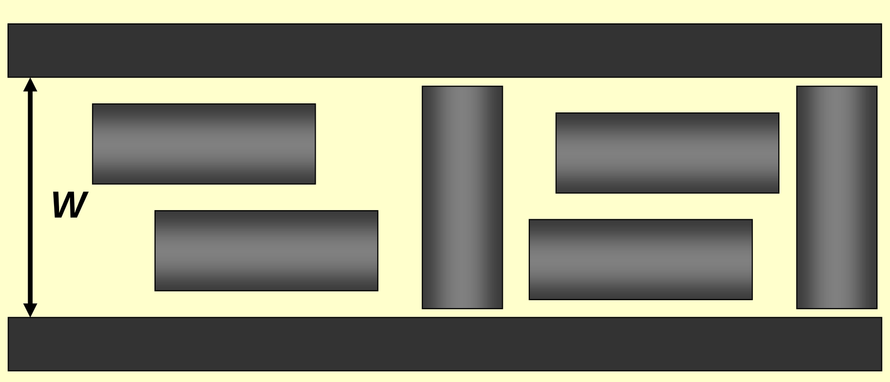
$$\beta G / N = -\ln Q_{NPT} = \beta P L + \ln(\beta P \Lambda)$$

Equation of state:

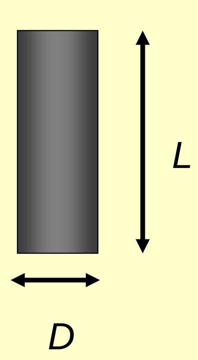
$$\beta P = \frac{\rho}{1 - \rho L}$$

L. Tonks: The complete equation of state of one, two and three dimensional gases of hard elastic spheres. Phys Rev 50: 955–963 (1936).

The case of nonzero thickness:



Hard rectangles are allowed to take only two orientations, but they are positionally free.

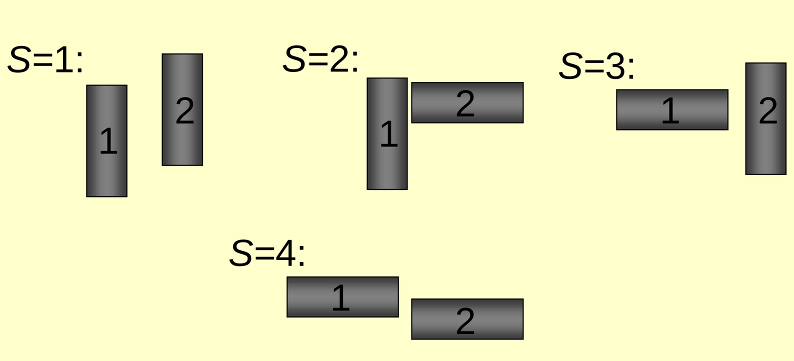


Only first and second neighbour interactions are allowed, i.e.

W<L+D and *W<3 D*

Using transfer matrix method one can derive an eigenvalue equation for a pair of neighboring rectangles in the following form

$$\sum_{S'=1}^{4} \int d(2) K_{S,S'}(1,2) \psi_{S',k}(2) = \lambda_k \psi_{S,k}(1), \quad S = 1,..,4$$



$$Q_{NPT} = Tr K^{N/2}$$

$$Q_{NPT} = \lambda_0^{N/2} \quad N \to \infty$$

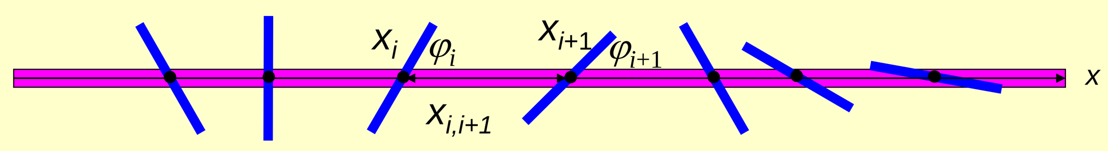
Planar ordering takes place at low densities, while homeotropic ordering at high densities

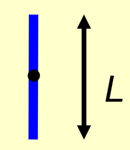
These calculations are still in progress.

Acknowledgement:

We acknowledge the financial support of the Hungarian State and the European Union under the TAMOP-4.2.2.A-11/1/KONV-2012-0071.

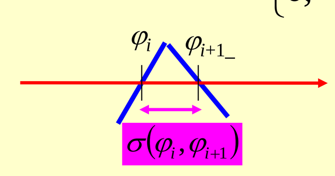
Freely rotating hard needles





Pair potential: $u(x_{i,i+1}, \varphi_i, \varphi_{i+1}) = \begin{cases} \infty, & x_{i,i+1} \le \sigma(\varphi_i, \varphi_{i+1}) \\ 0, & x_{i,i+1} > \sigma(\varphi_i, \varphi_{i+1}) \end{cases}$

where



Isobaric partition function:

$$Q_{NPT} = \frac{1}{\Lambda^N} \int dx_1 d\varphi_1 ..dx_N d\varphi_N \exp\left(-\beta \sum_{i=1}^{N} \left(u(x_{i,i+1}, \varphi_i, \varphi_{i+1}) + P x_{i,i+1}\right)\right)$$

$$x_i \to x_{i,i+1} \quad \Rightarrow \quad Q_{NPT} = \frac{1}{\Lambda^N} \int_{\sigma(\varphi_1,\varphi_2)}^{\infty} dx_{1,2} d\varphi_1 ... \int_{\sigma(\varphi_N,\varphi_1)}^{\infty} dx_{N,1} d\varphi_N \exp(-\beta P x_{1,2}) ... \exp(-\beta P x_{N,N+1})$$

$$Q_{NPT} = \left(\frac{1}{\Lambda}\right)^N \int d\varphi_1 ..d\varphi_N K(\varphi_1,\varphi_2) K(\varphi_2,\varphi_3) ... K(\varphi_N,\varphi_1) \qquad K(\varphi_i,\varphi_{i+1}) = \frac{\exp(-\beta P \sigma(\varphi_i,\varphi_{i+1}))}{\beta P}$$

Matrix product:

$$K^2(\varphi_i,\varphi_{i+2}) = \int d\varphi_{i+1} K(\varphi_i,\varphi_{i+1}) K(\varphi_{i+1},\varphi_{i+2}) \quad \Rightarrow \quad Q_{NPT} = \mathrm{Tr}\hat{K}^N = \int d\varphi\, K^N(\varphi,\varphi)$$

$Q_{NPT} = \sum_{k=0}^{\infty} \lambda_k^N$ **where** $\int d\varphi_1 K(\varphi,\varphi_1) \psi_k(\varphi_1) = \lambda_k \psi_k(\varphi)$ **Eigenvalue-equation**

$$Q_{NPT} = \sum_{k=0}^{\infty} \lambda_k^N = \lambda_0^N \left(1 + (\lambda_1/\lambda_0)^N + ...\right) \quad \lambda_0 > \lambda_1 > \lambda_2 > .....$$

$$Q_{NPT} = \lambda_0^N \quad N \to \infty$$

Orientational distribution function (ODF):

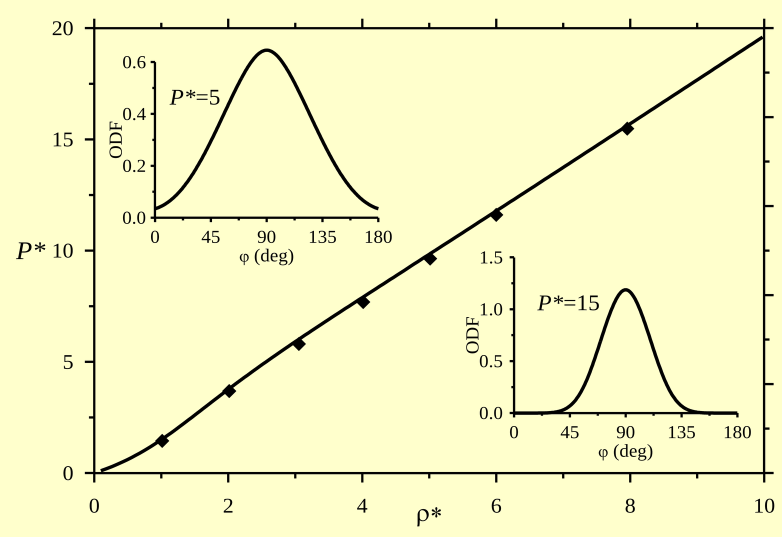
$$f(\varphi) = \psi_0^2(\varphi)$$

Equation of state:

$$\frac{1}{\rho} = -\frac{\partial \log \lambda_0}{\partial P}$$

$\rho^* = \rho L$

$P^* = \beta P L$

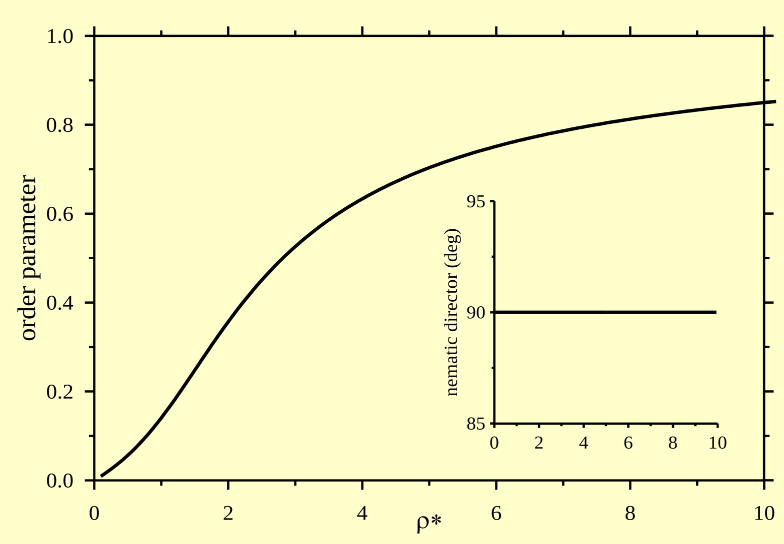


Orientational order parameter:

$$S = \sqrt{\langle \sin(2\varphi) \rangle^2 + \langle \cos(2\varphi) \rangle^2}$$

Nematic director:

$$\tan\varphi_d = \frac{S - \langle \cos(2\varphi) \rangle}{\langle \sin(2\varphi) \rangle}$$



Orientational order parameter:

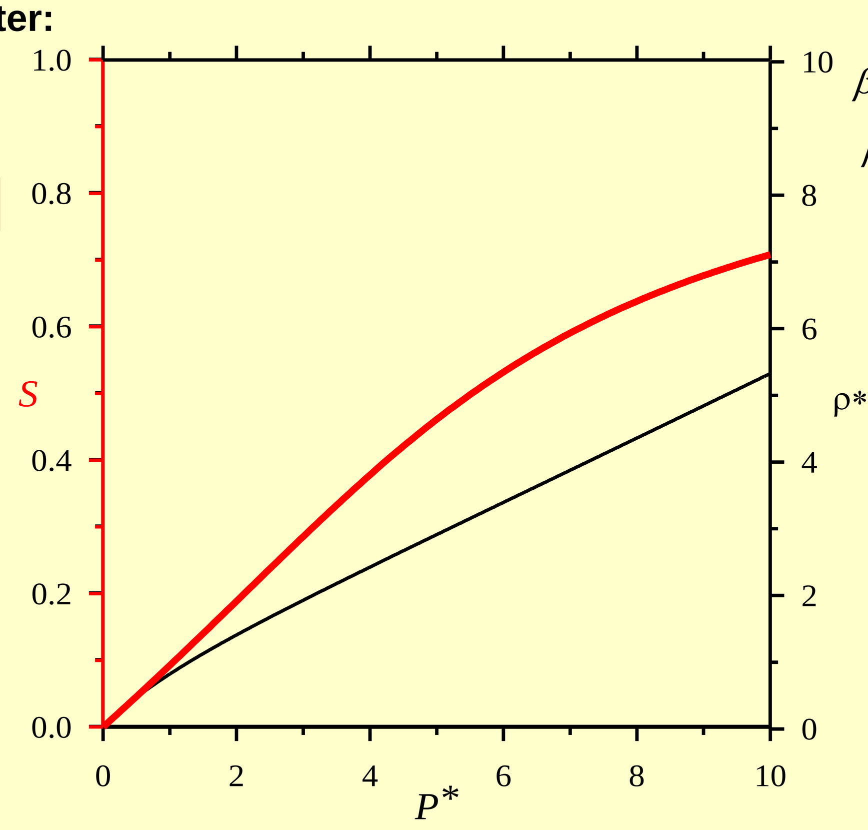
$S(P \to 0) = 0$

$S(P \to \infty) = 1$

Equation of state:

$\beta P = \rho \quad \rho \to 0$

$\beta P = 2\rho \quad \rho \to \infty$



Exact results for approximate contact distance

$$\sigma(\varphi,\varphi') \approx l|\varphi - \varphi'|/\pi$$

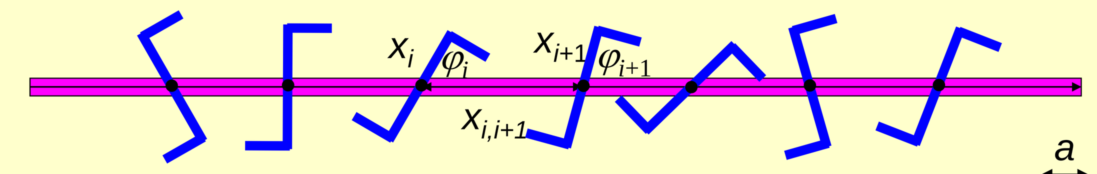
$$\lambda_i = \frac{2\pi}{P^{*2} + \kappa_i^2} \qquad \psi_{2j}(\varphi) = \sqrt{\frac{2\kappa_{2j}}{\pi(\kappa_{2j} + \sin\kappa_{2j})}} \cos\left(\frac{\kappa_{2j}}{\pi}(\varphi - \pi/2)\right)$$

$$\kappa_{2j} \tan(\kappa_{2j}/2) = P^*$$

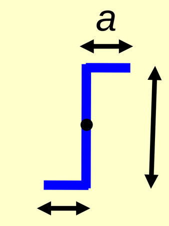
$$\rho^{*-1} = \frac{2(P^* + \kappa_0 \kappa_0)}{P^{*2} + \kappa_0^2} \qquad \psi_{2j+1}(\varphi) = \sqrt{\frac{2\kappa_{2j+1}}{\pi(\kappa_{2j+1} - \sin\kappa_{2j+1})}} \sin\left(\frac{\kappa_{2j+1}}{\pi}(\varphi - \pi/2)\right)$$

$$S = \frac{\kappa_0^2 \sin\kappa_0}{(\pi^2 - \kappa_0^2)(\kappa_0 + \sin\kappa_0)} \qquad -\kappa_{2j+1}/\tan(\kappa_{2j+1}/2) = P^*$$

Freely rotating hard zigzag needles



$L = 2a + b$



Transfer-matrix equations:

$$\int d\varphi_1 K(\varphi,\varphi_1) \psi_k(\varphi_1) = \lambda_k \psi_k(\varphi)$$

$$K(\varphi_1,\varphi_2) = \sum_{i=1}^{3} (-1)^{i+1} \exp(-\beta P \sigma_i(\varphi_1,\varphi_2)) / \beta P$$

$$Q_{NPT} = \sum_{k=0}^{\infty} \lambda_k^N \qquad Q_{NPT} = \lambda_0^N \quad N \to \infty$$

Orientational distribution function (ODF):

$$f(\varphi) = \psi^2(\varphi)$$

Equation of state:

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$\rho^* = \rho L$

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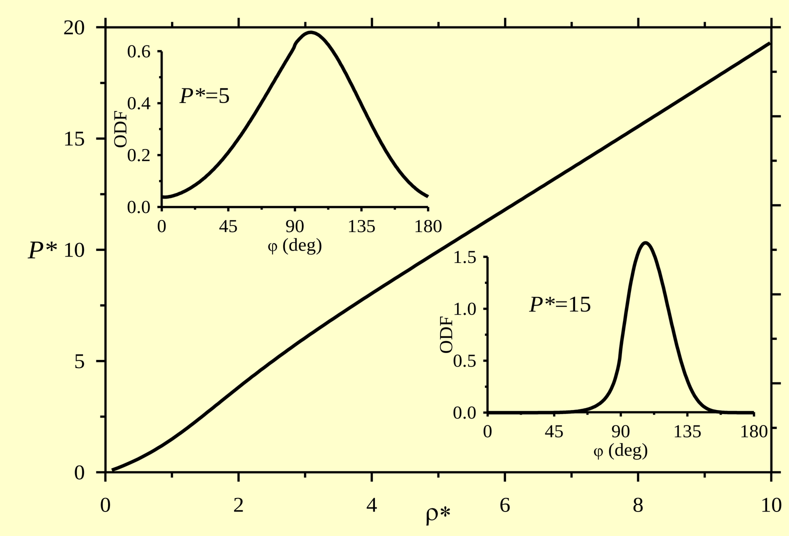

Orientational order parameter:

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Nematic director:

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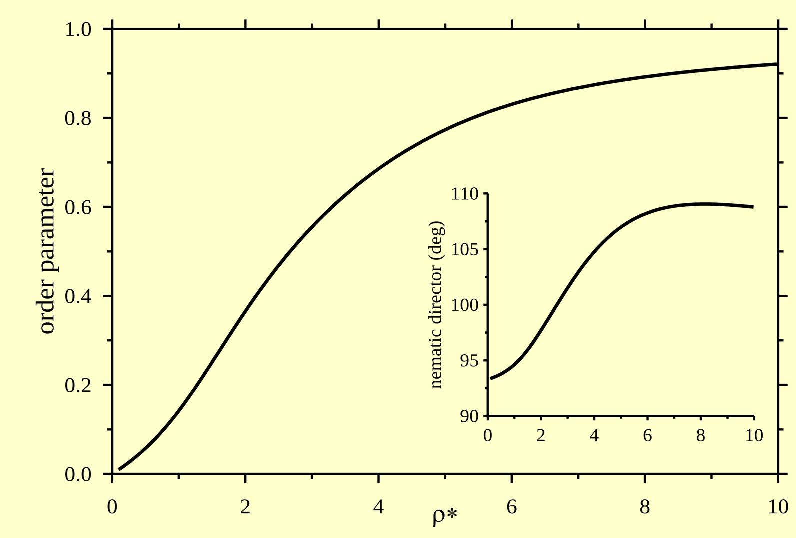
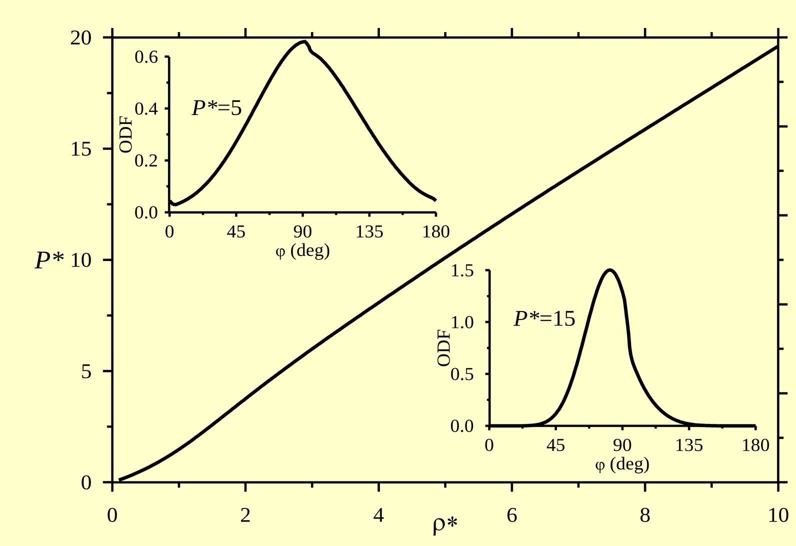
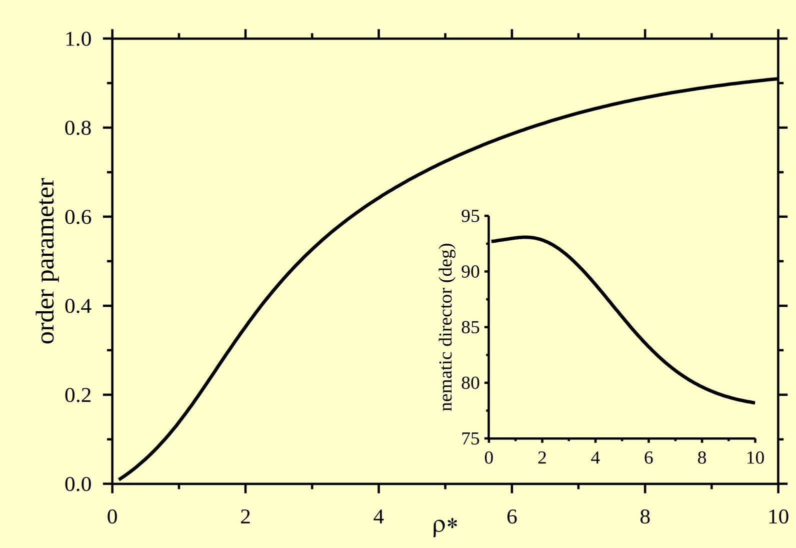


***a*/*L*=0.025**

Equation of state and orientational distribution function



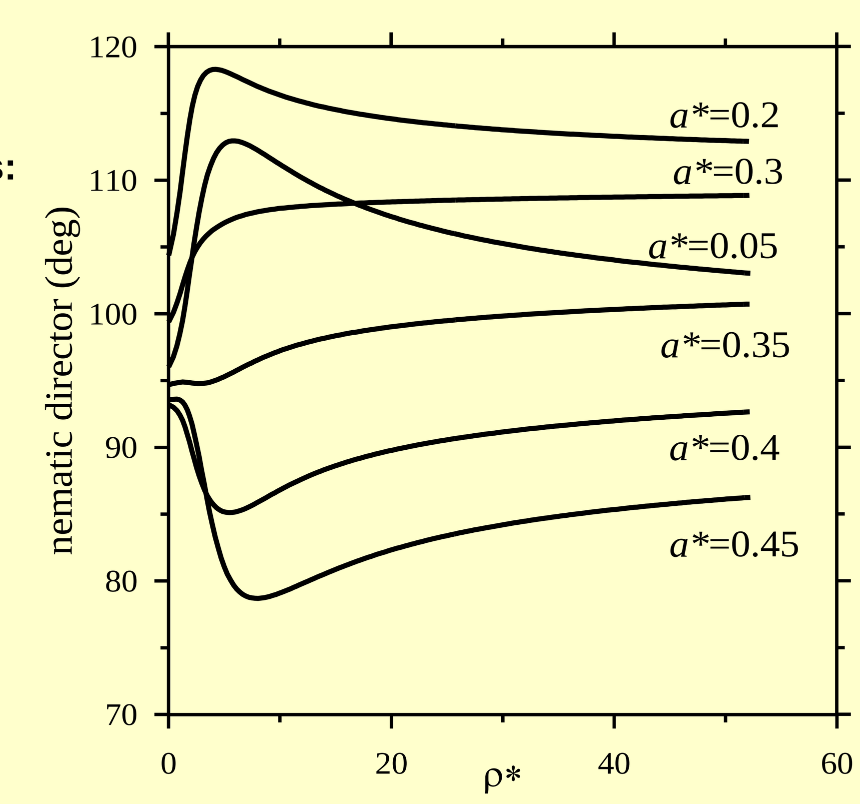
Orientational order parameter and nematic director



***a*/*L*=0.475**

Nematic director at different tail lengths:

a**=*a*/*L



Conclusion: The zig-zag shape gives rise to peculiar density dependence on the nematic director, i.e. the system form a tilted smectic C layer.