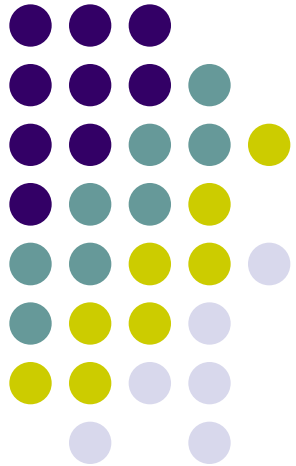
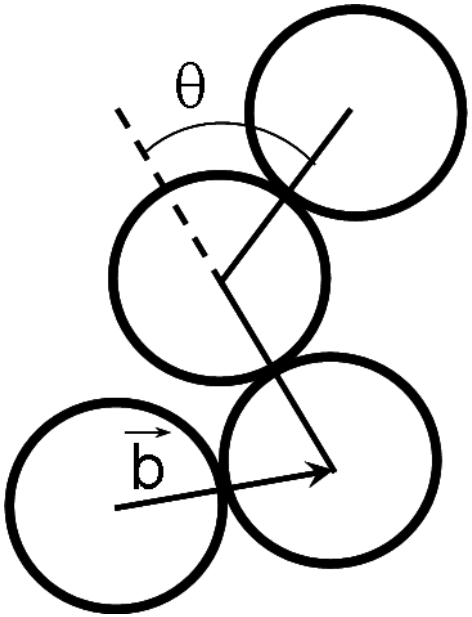
Wang-Landau type Monte Carlo study of crystallization in melts of short semi-flexible polymers



Timur Shakirov

University of Halle

Computational model



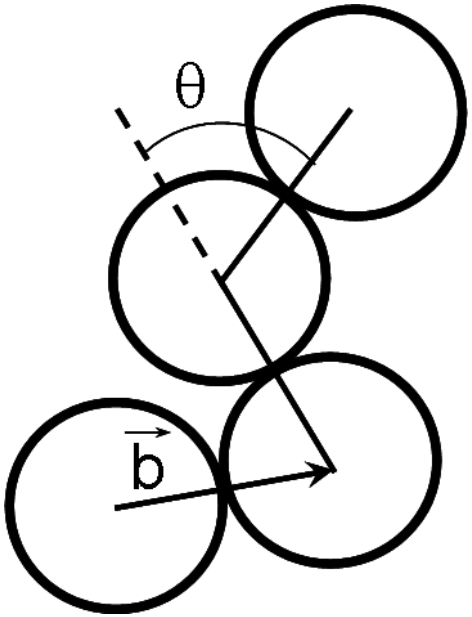
Hard spheres

+

$$U(\theta)=\begin{cases}-\varepsilon & \theta<\theta_{\max}\\ 0 & \theta>\theta_{\max}\end{cases}$$

$$0\le\theta\le 120^{\circ}$$

Computational model



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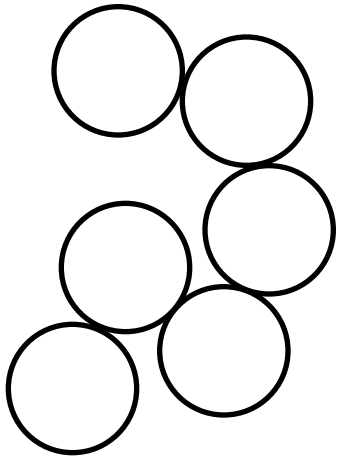
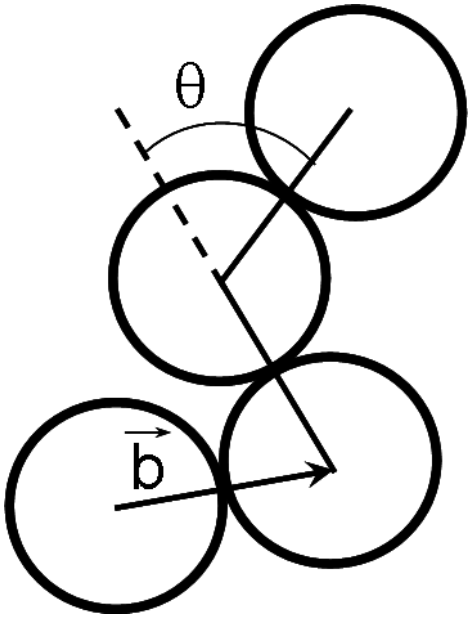
High Energies



Computational model



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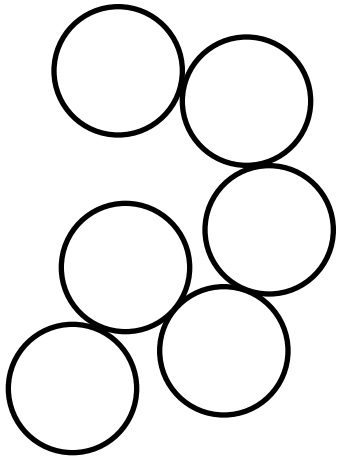
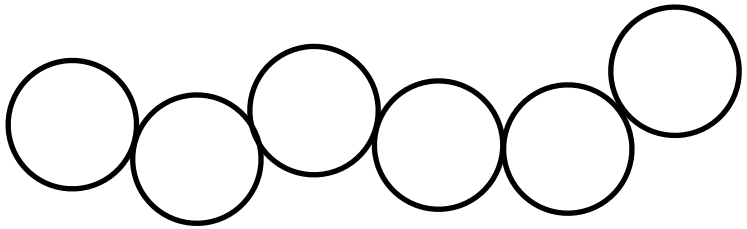
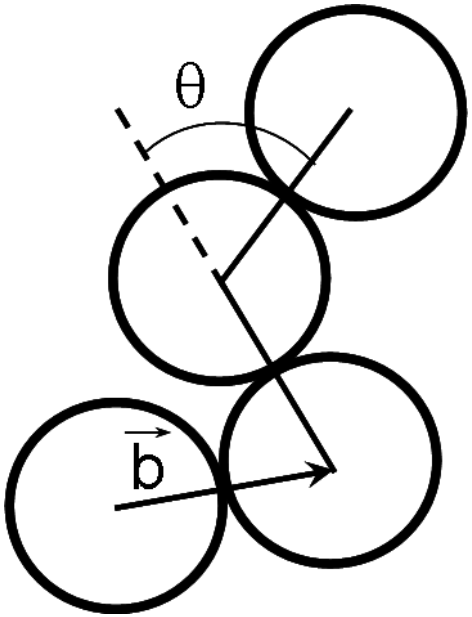


Low Energies



Computational model



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"Ideal" chains

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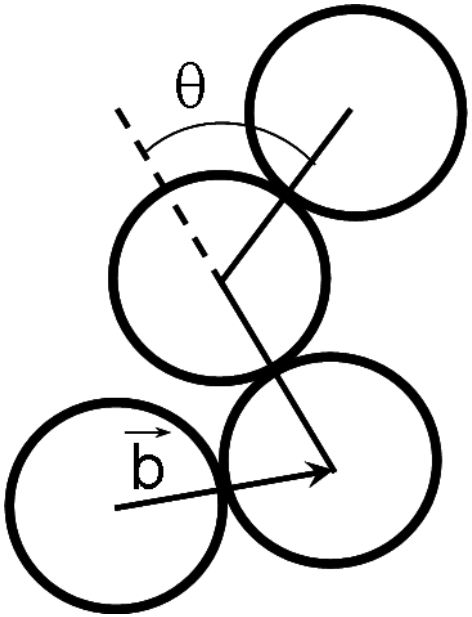
Computational model



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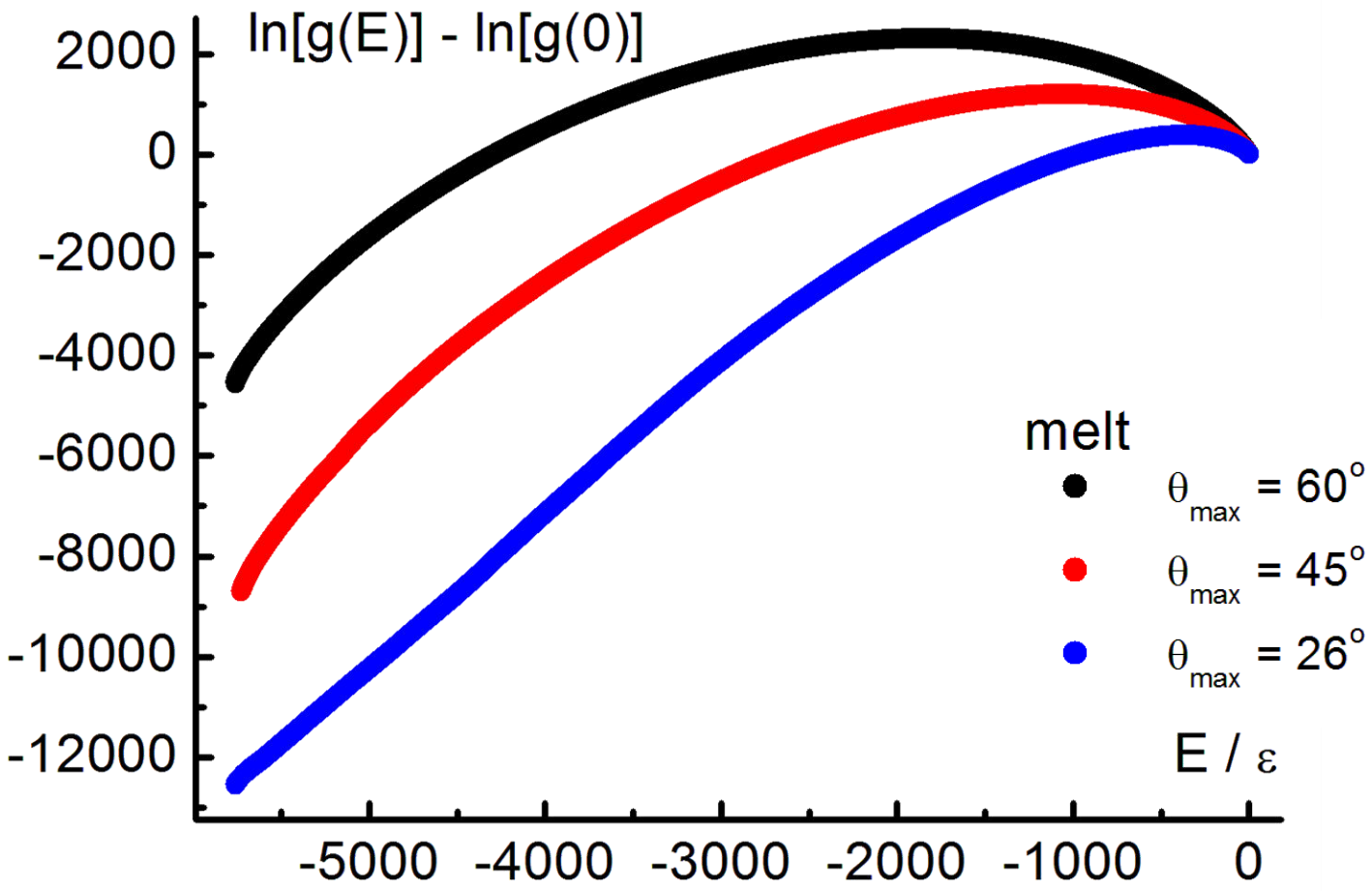
"Ideal" chains

$$U(\theta)=\begin{cases}-\varepsilon & \theta<\theta_{\max}\\ 0 & \theta>\theta_{\max}\end{cases}$$

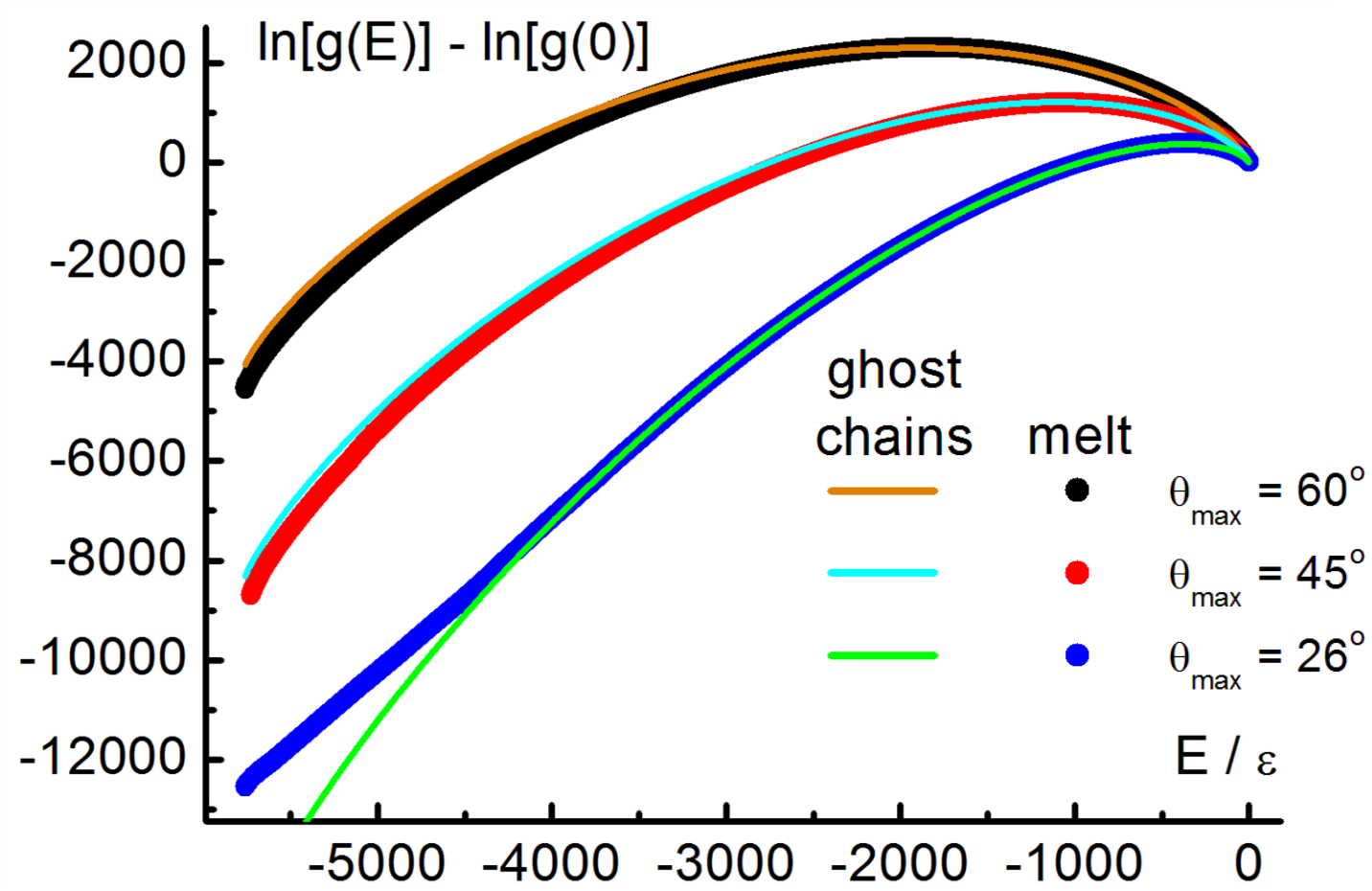
$$\hat{g}(E)\propto\binom{N_E}{|E|}p^{|E|}(1-p)^{N_E-|E|}$$

$$0\le\theta\le 120^{\circ}$$

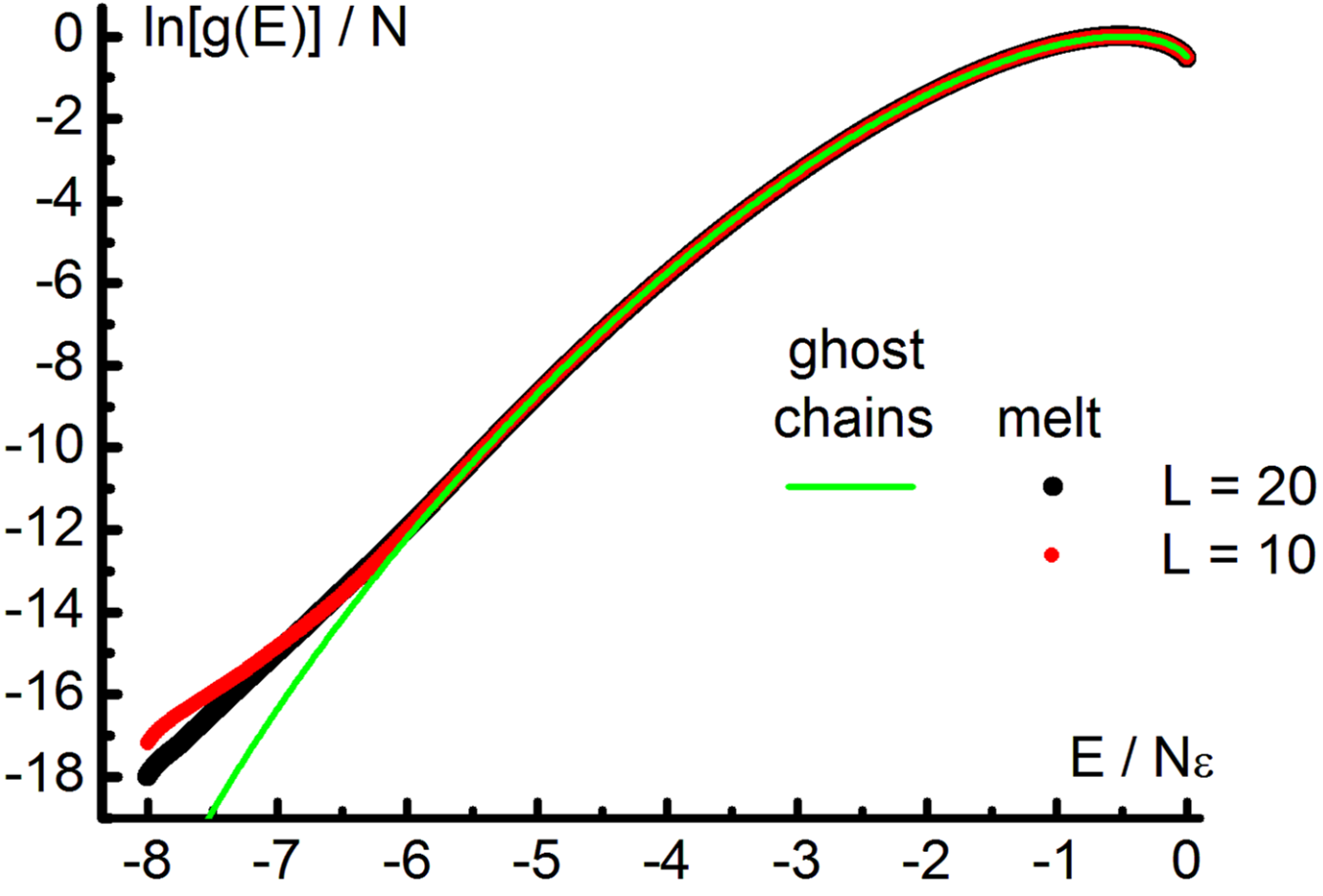
Density of states



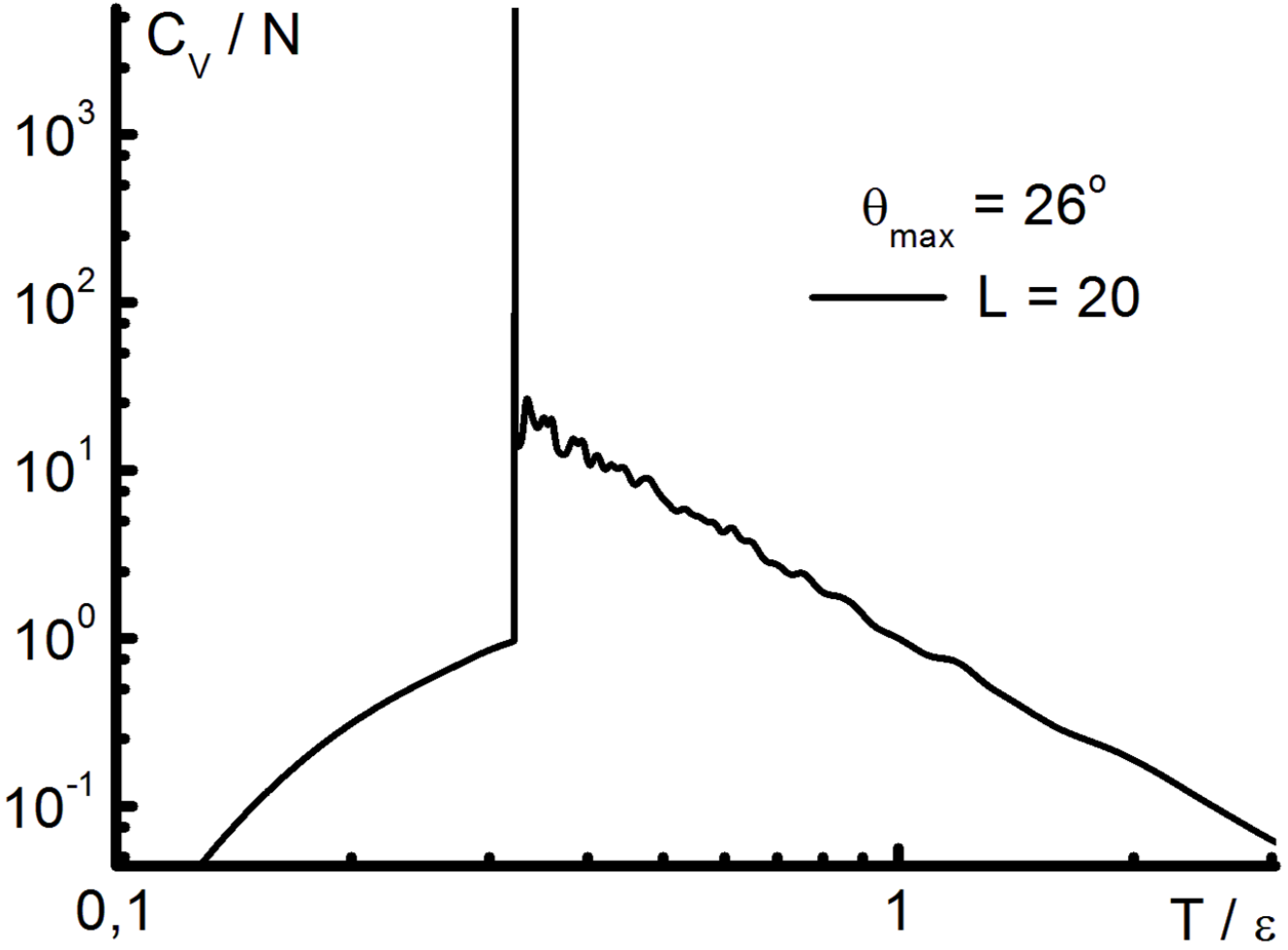
Density of states



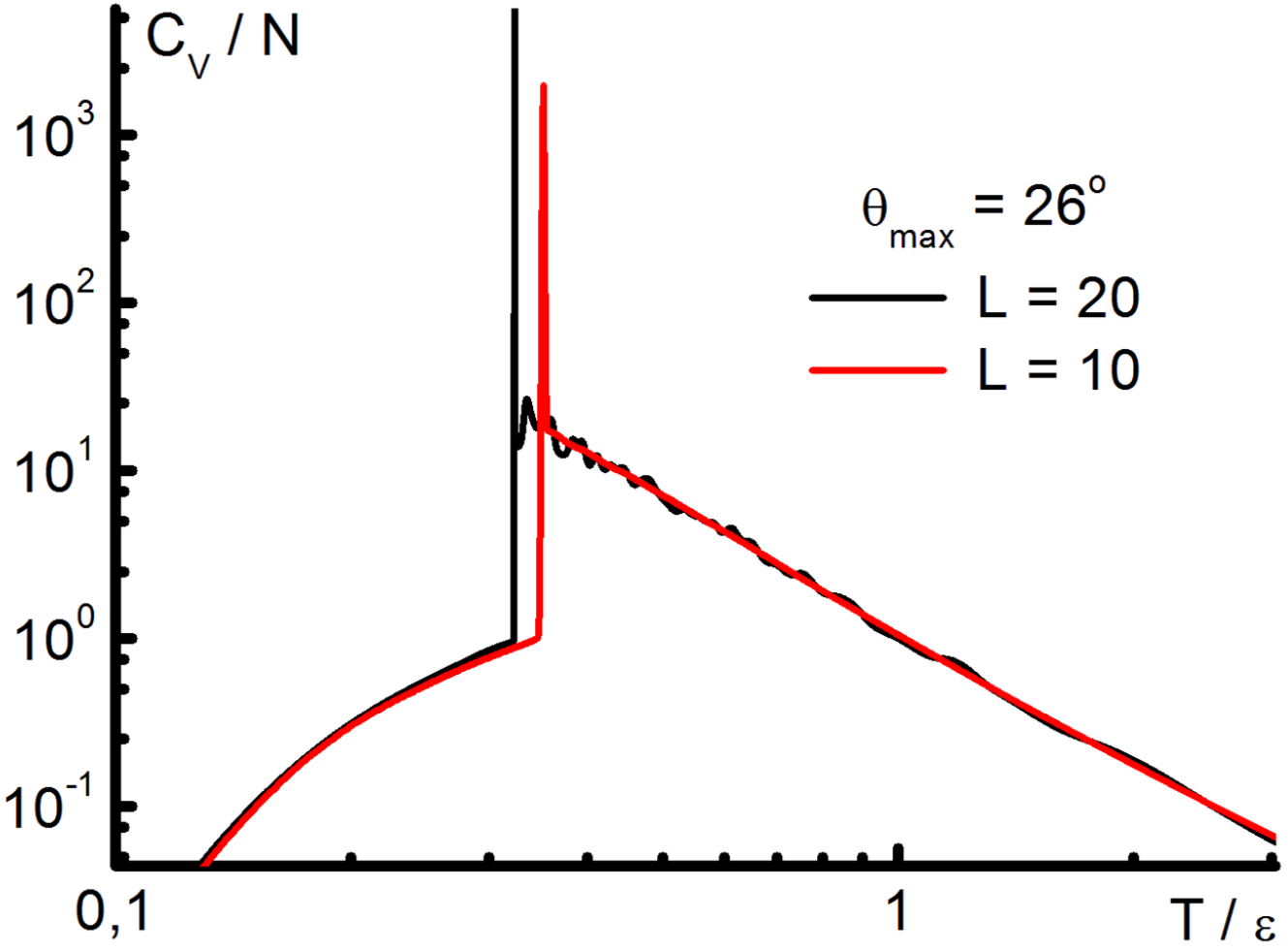
Density of states. Stiff chains



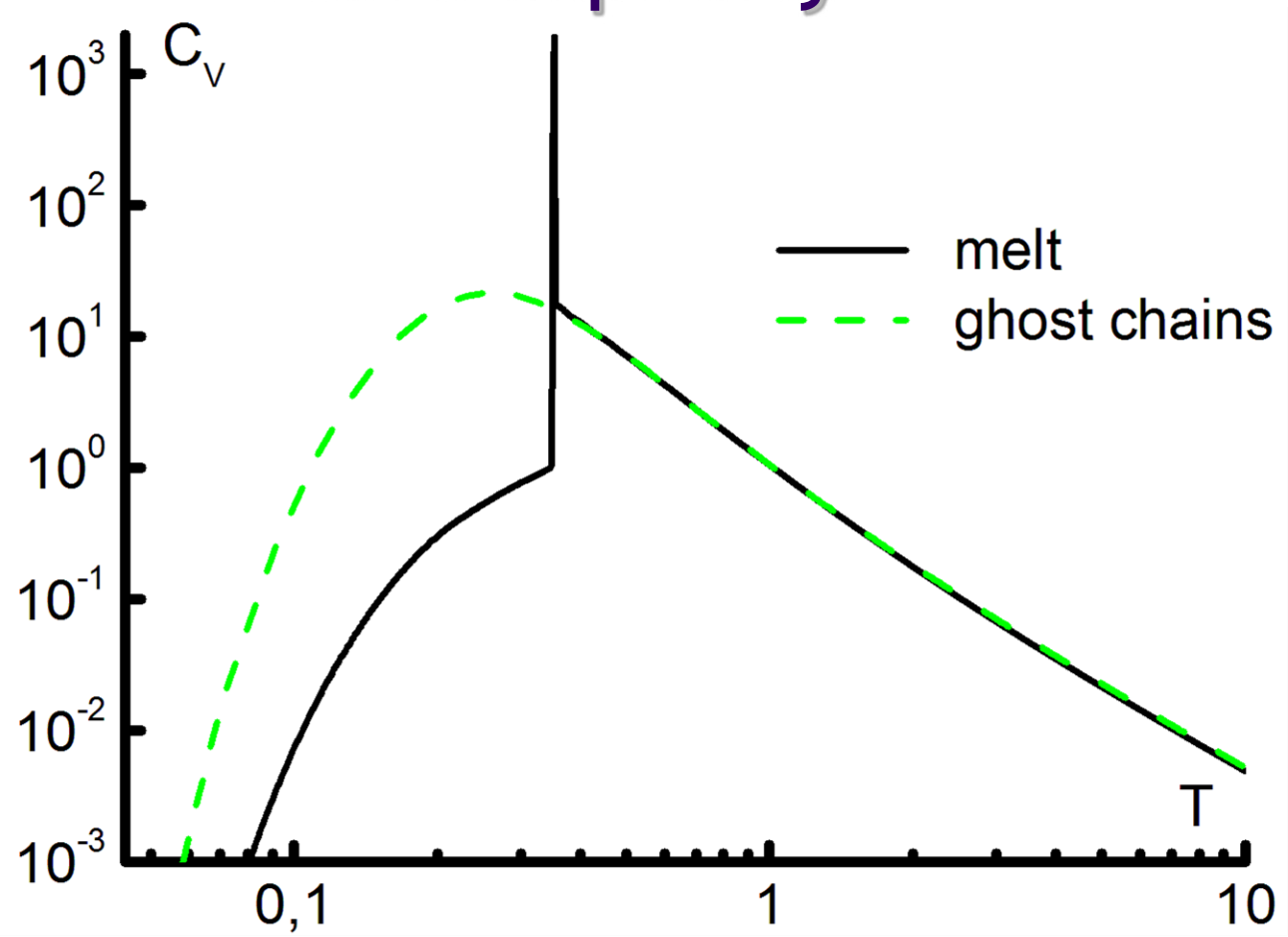
Size effects. Heat capacity



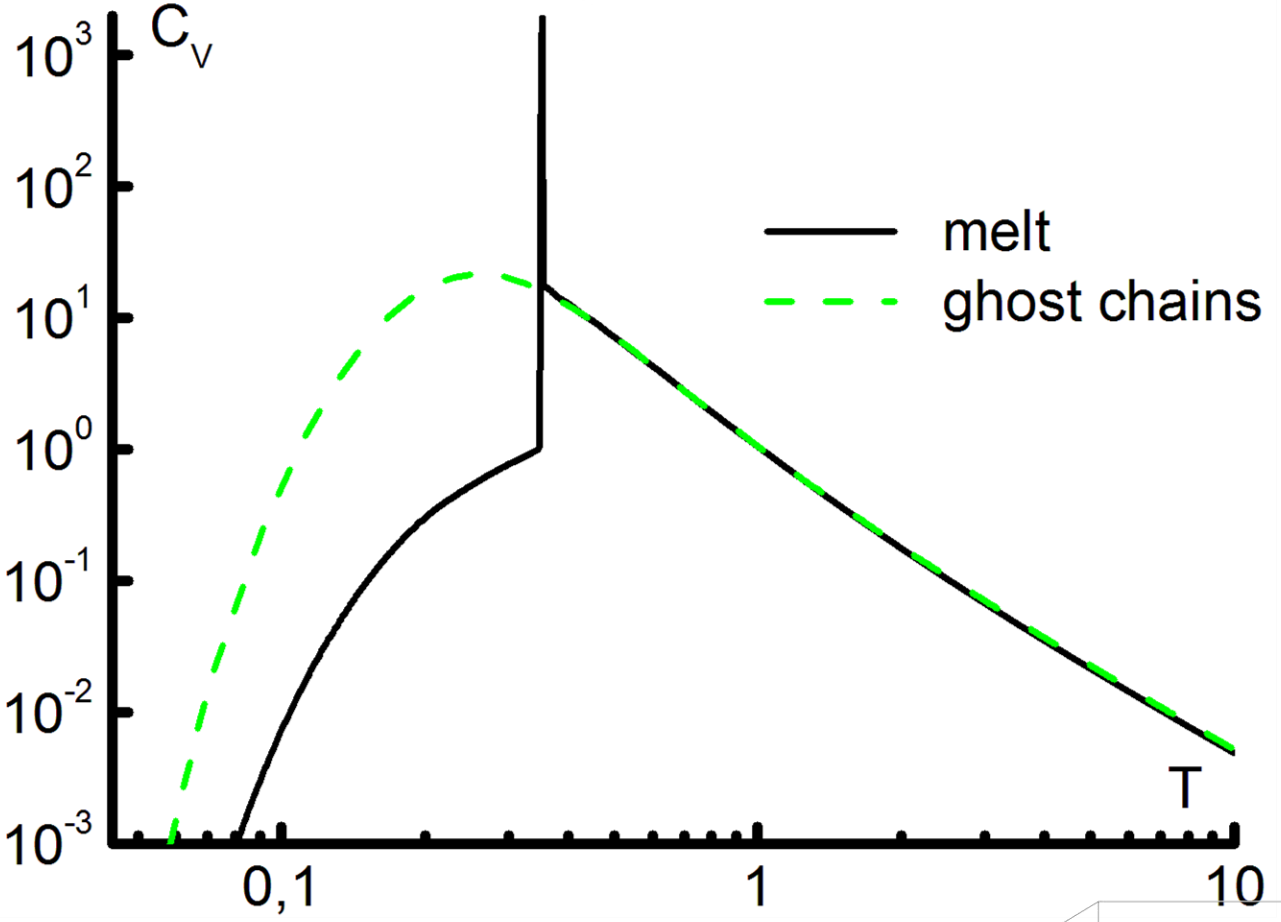
Size effects. Heat capacity

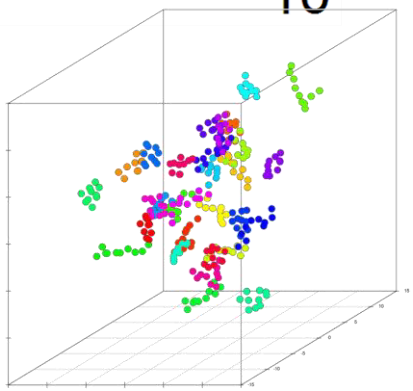


Heat capacity

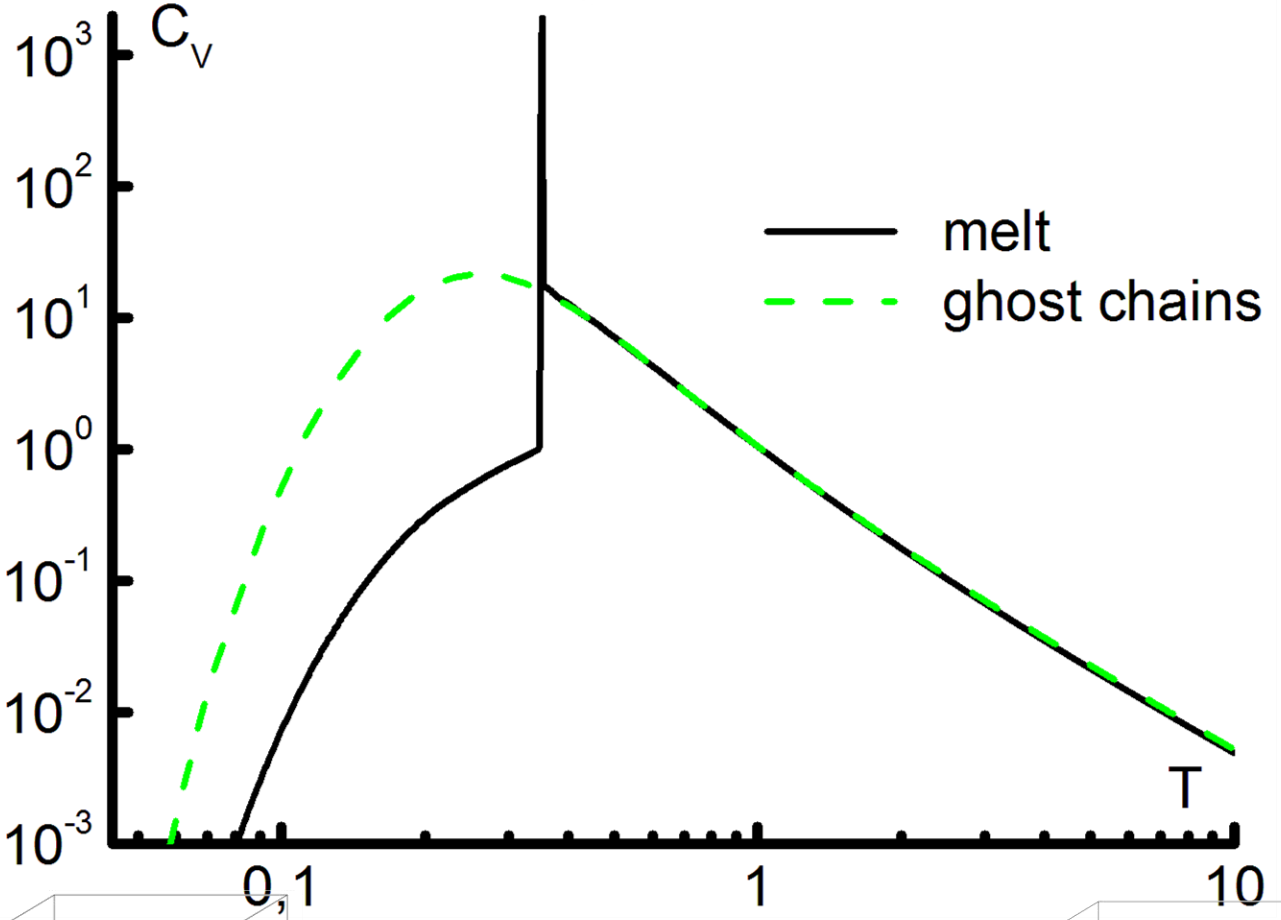


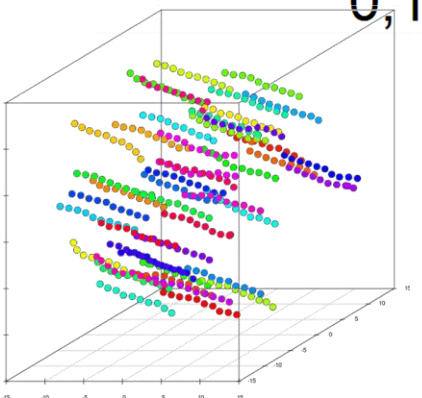
Heat capacity

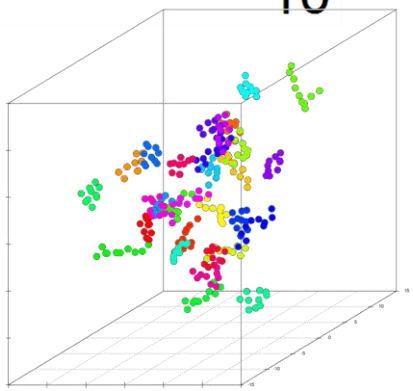




Heat capacity

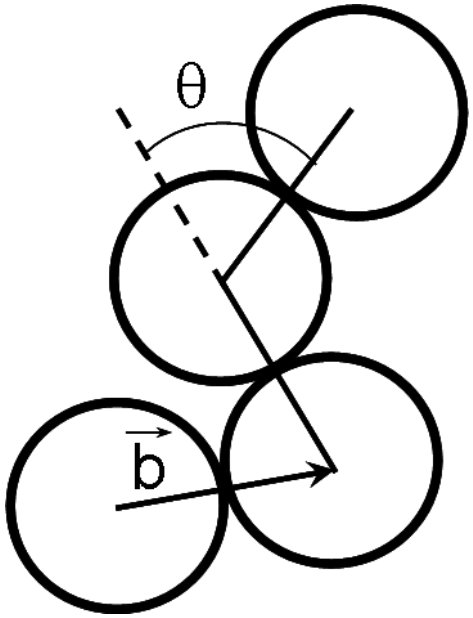






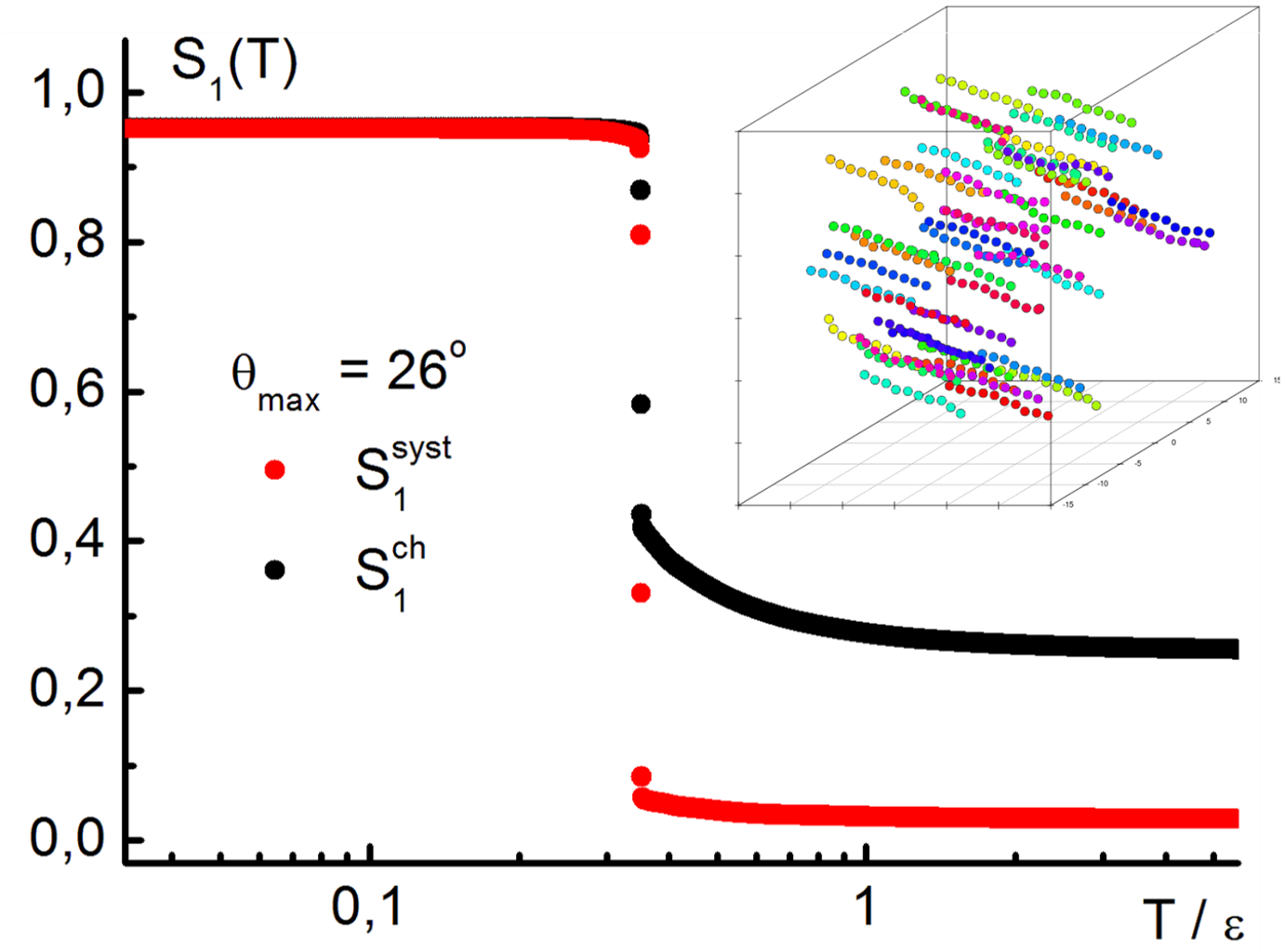
Order parameter. Definition

$$Q_{\alpha\beta} = \frac{1}{N}\sum_i \frac{3b_{i\alpha}b_{i\beta} - \delta_{\alpha\beta}}{2}$$

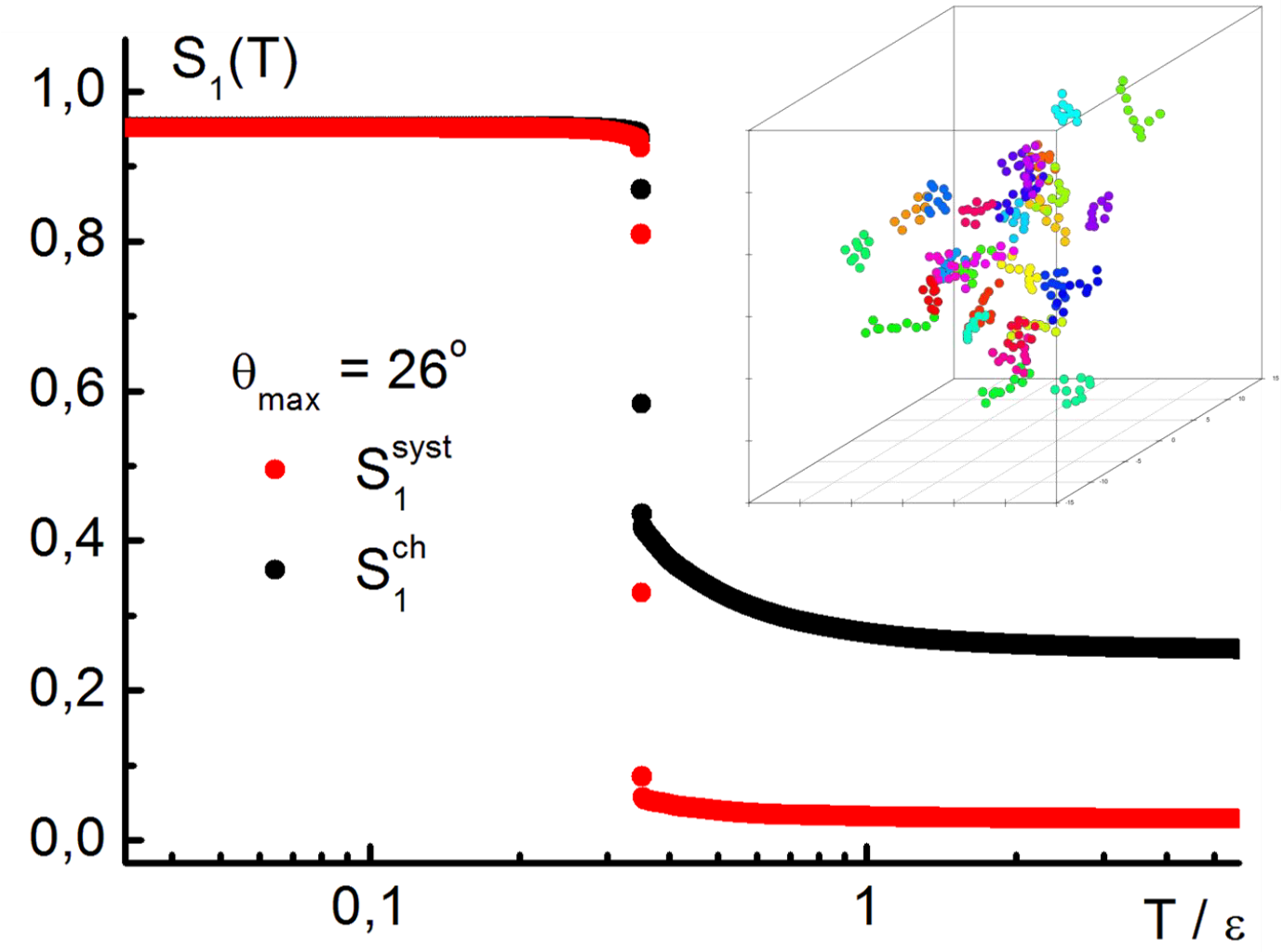


$$S_1 = \max(\det(Q_{\alpha\beta} - S_i\delta_{\alpha\beta}) = 0)$$

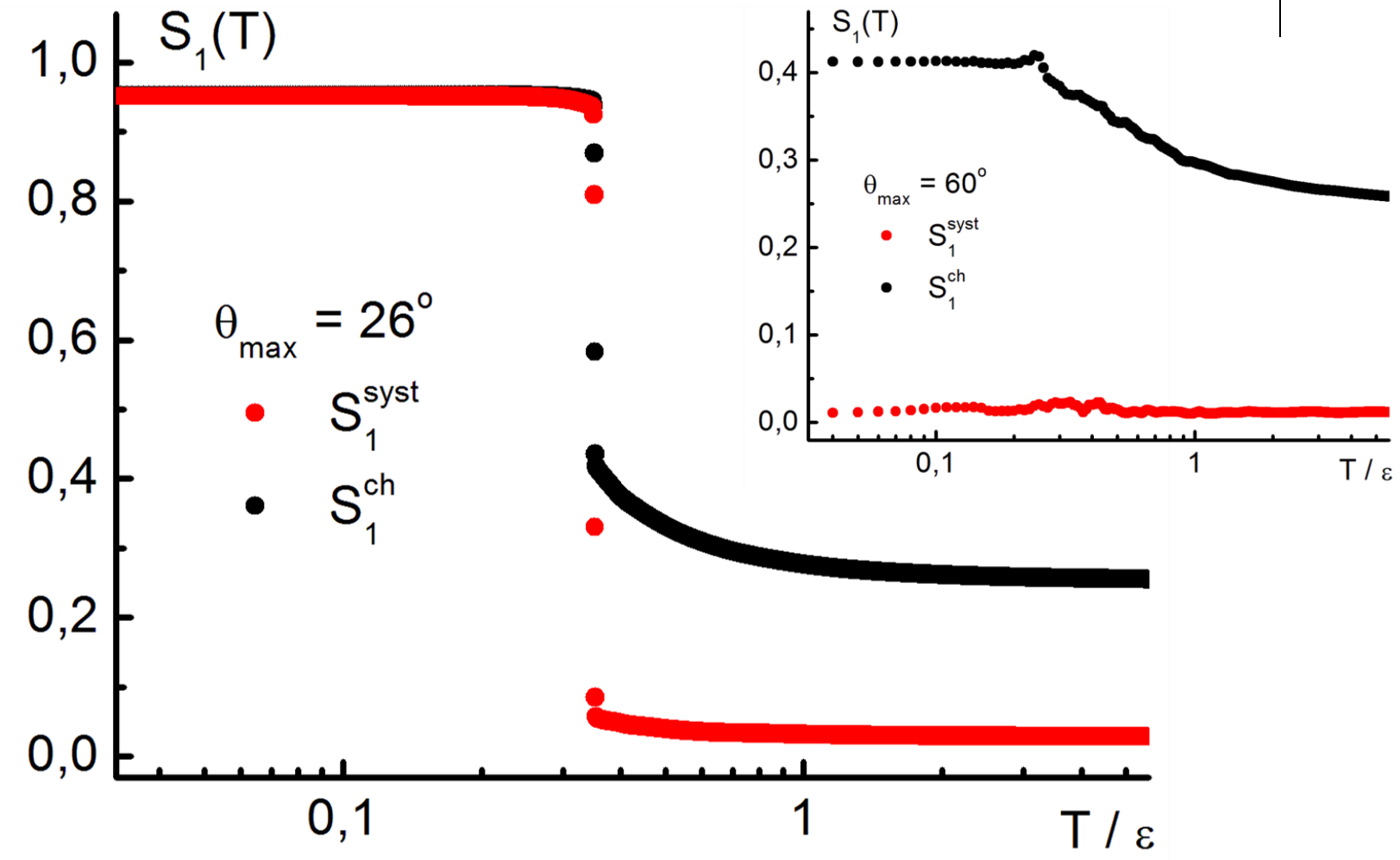
Order parameter. Temperature dependence



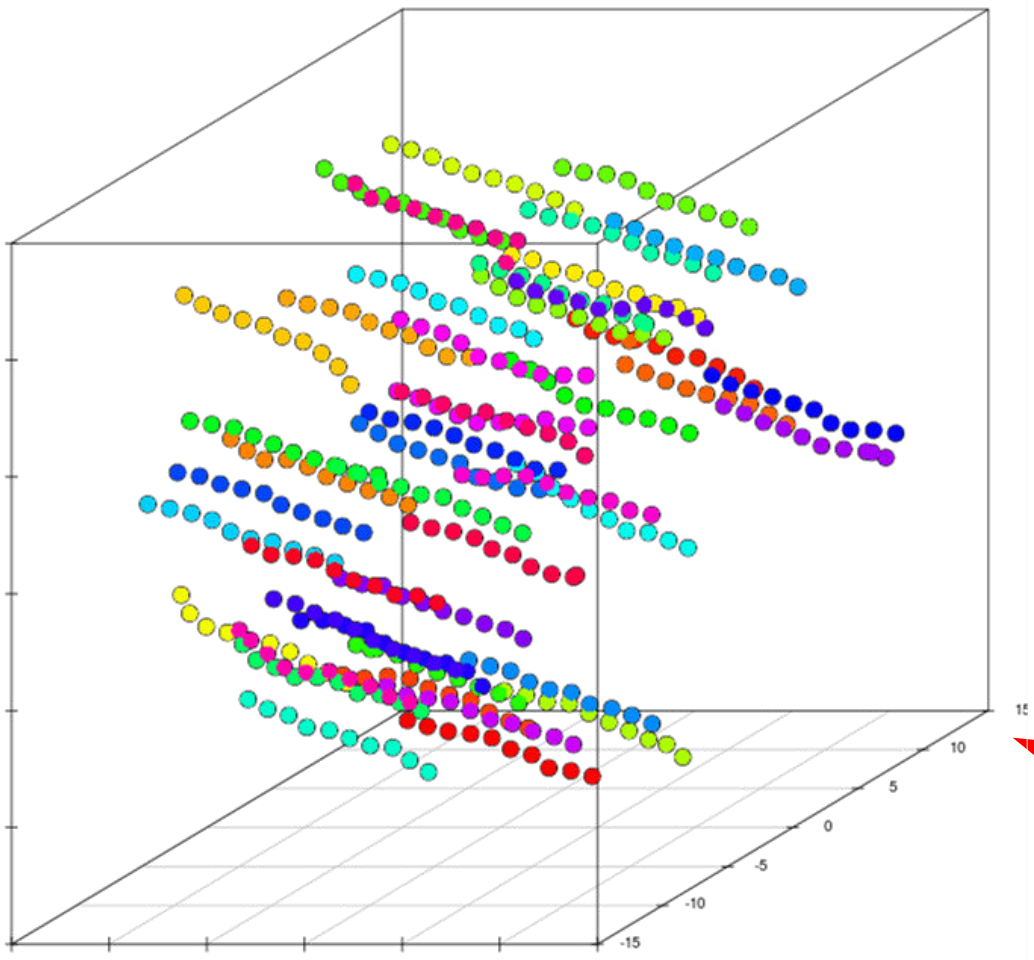
Order parameter. Temperature dependence



Order parameter. Temperature dependence



Order parameter and density distribution

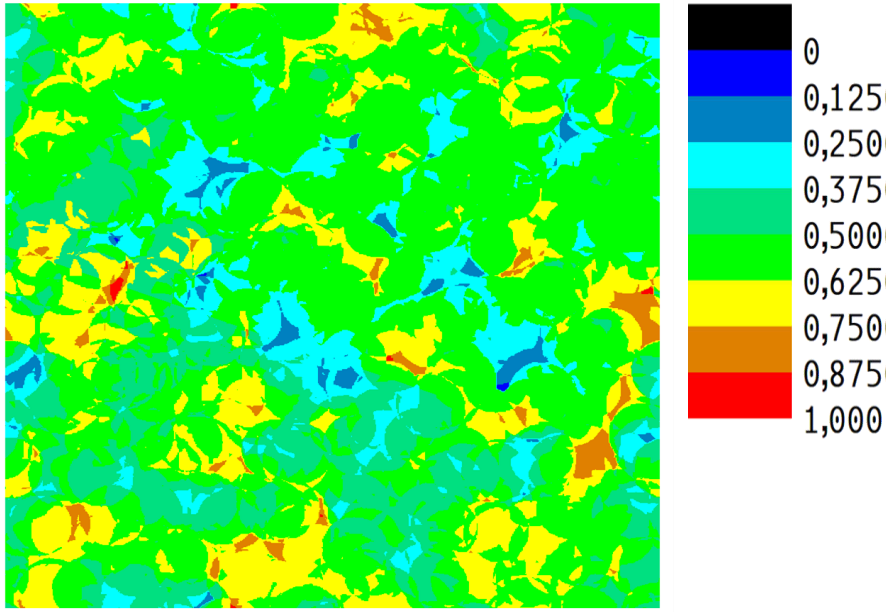


$$\left| \left(\vec{n}_S \cdot \vec{b} \right) \right|$$

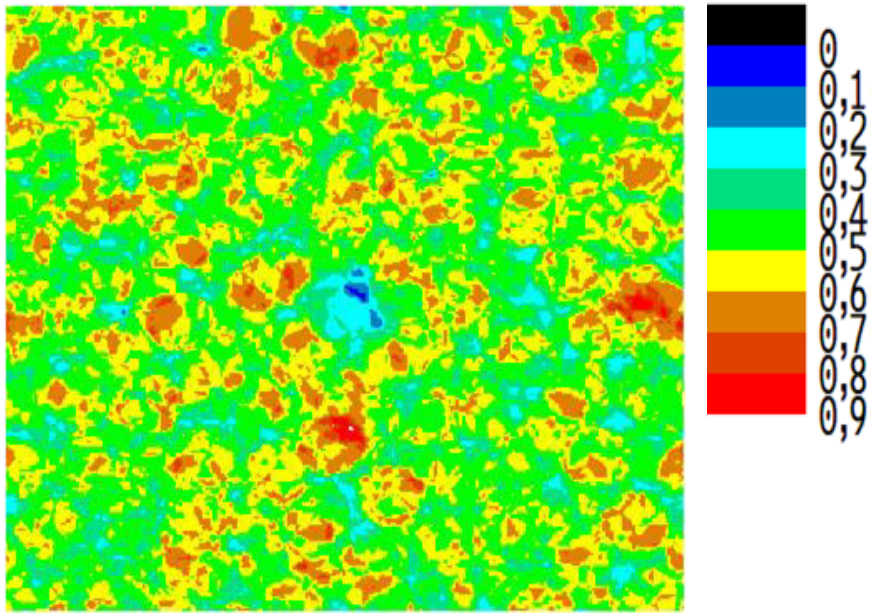
$\vec{n}_S$

Order parameter and density distributions. High energies

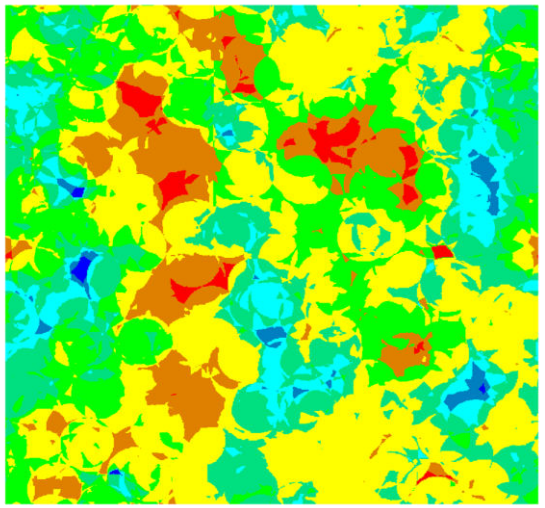
Orientation

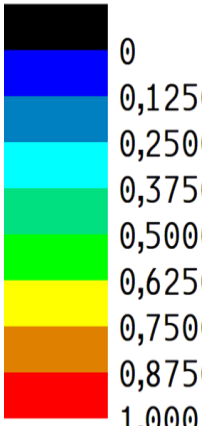


Density

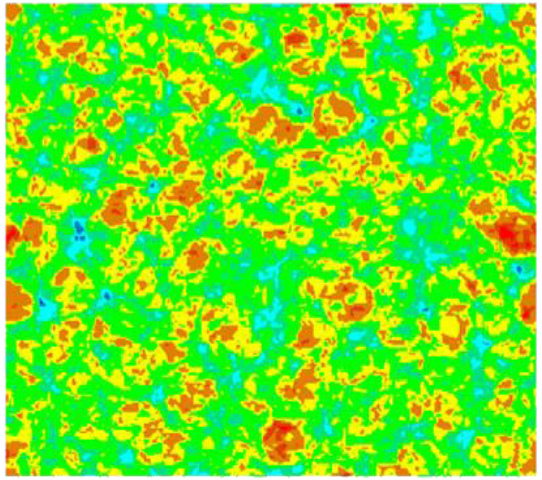


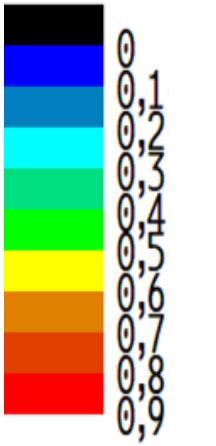
Order parameter and density distributions. Phase transition



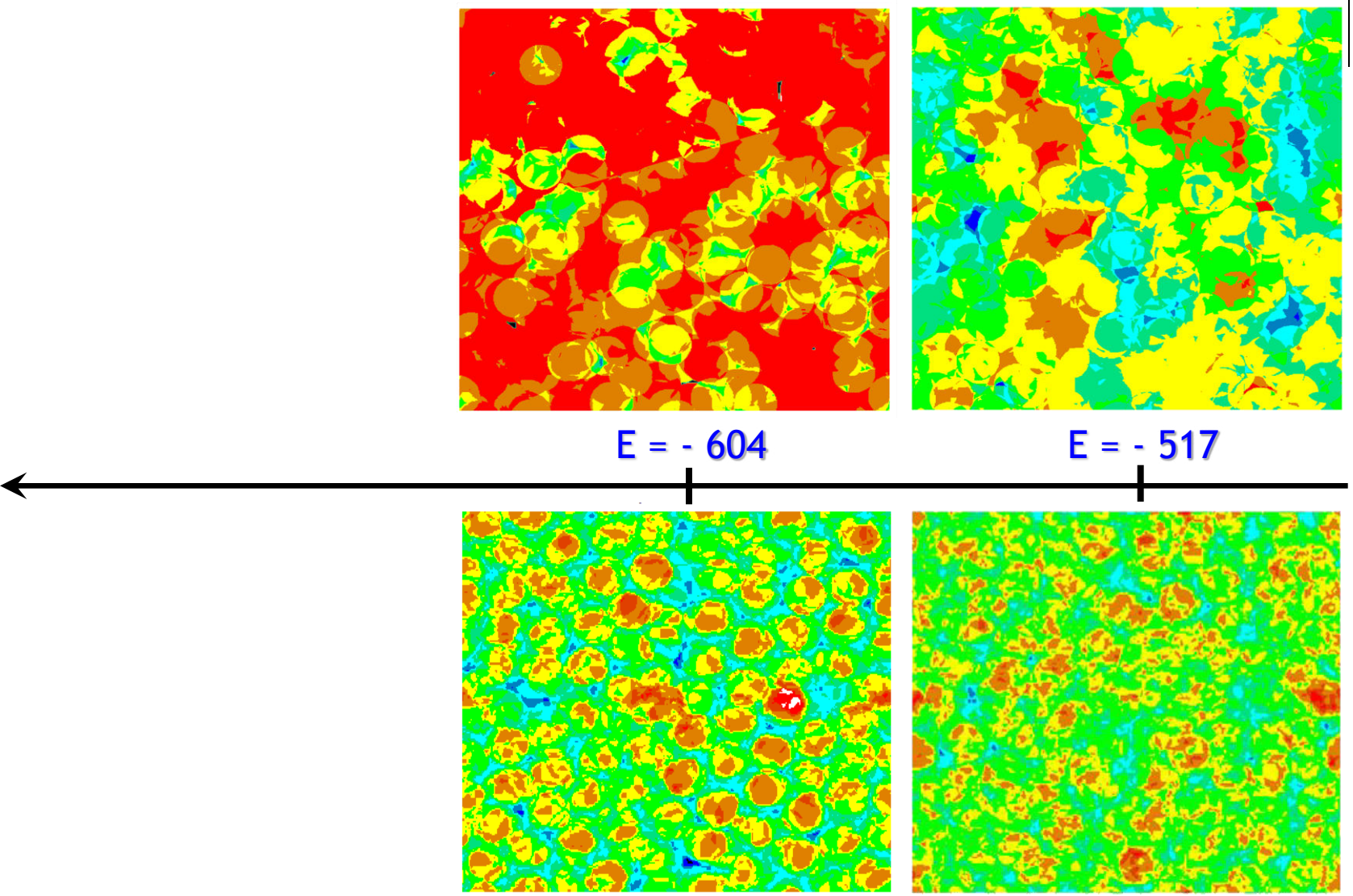


E = - 517

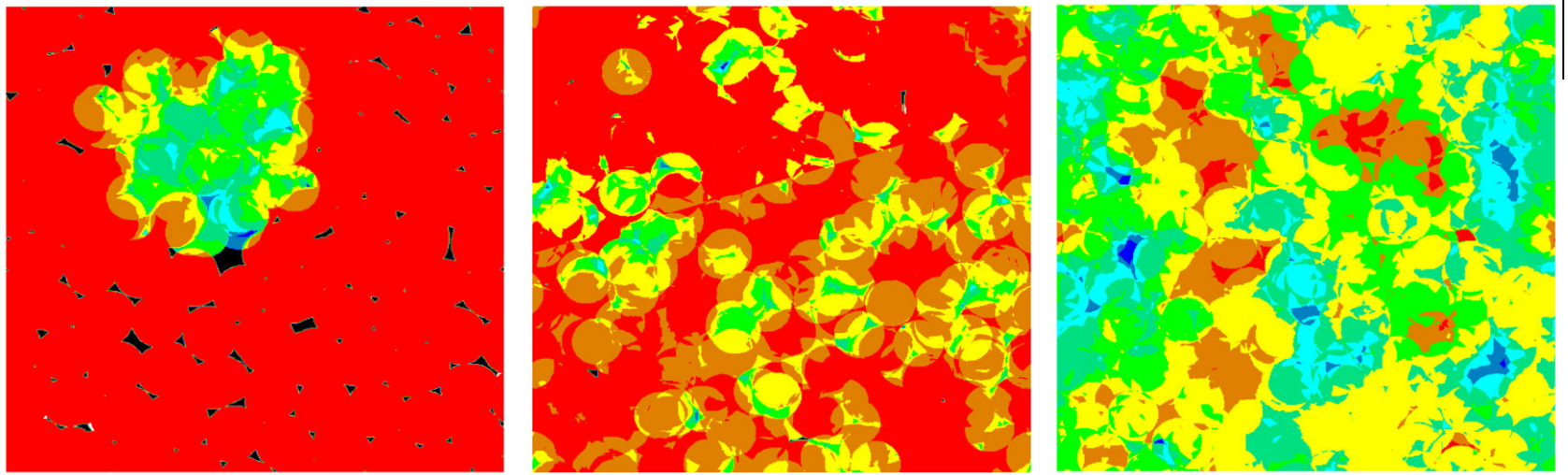




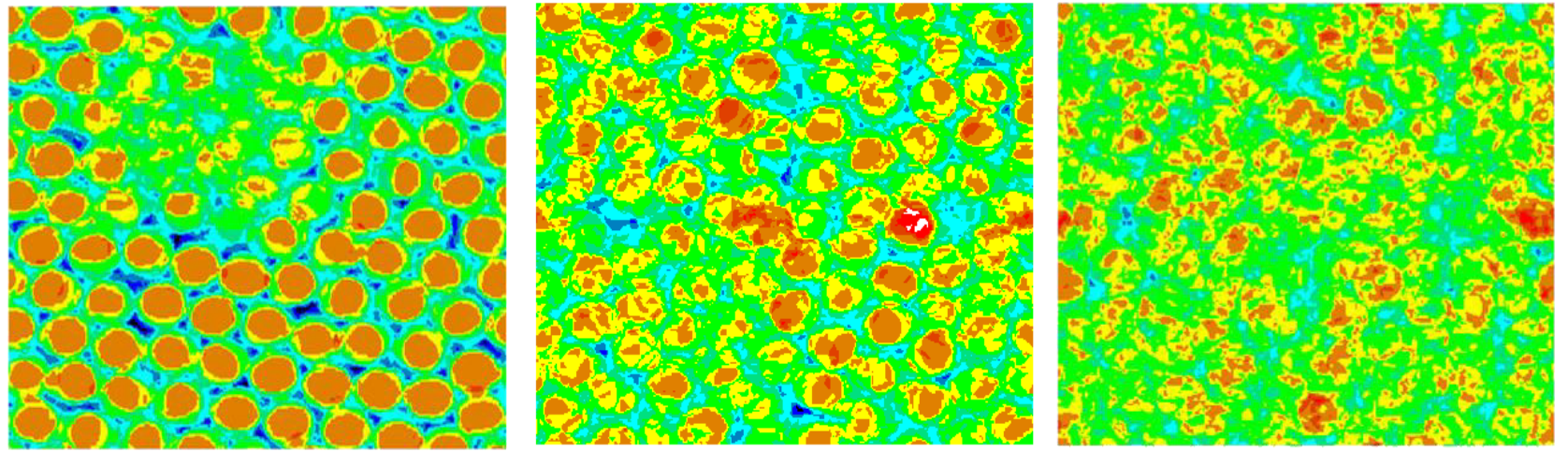
Order parameter and density distributions. Phase transition



Order parameter and density distributions. Phase transition

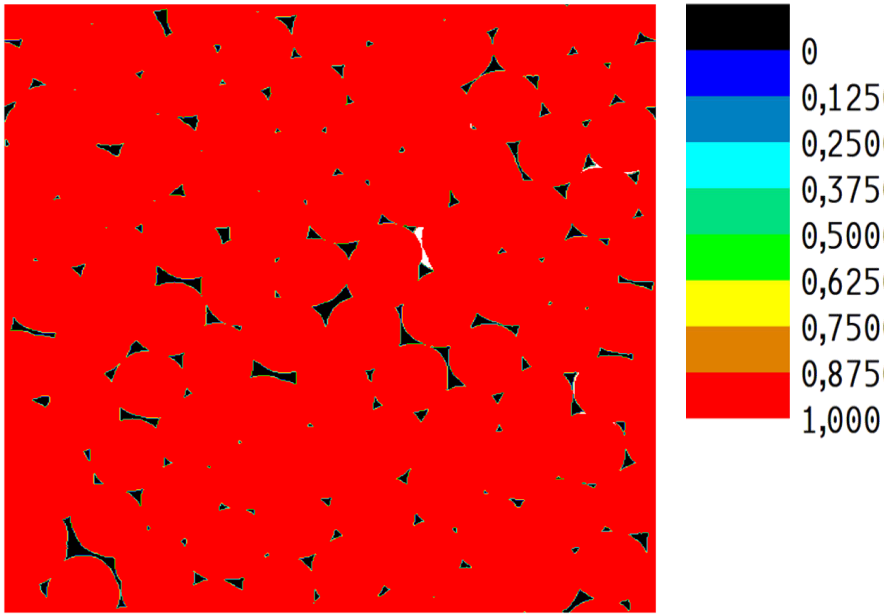


E = - 651 E = - 604 E = - 517

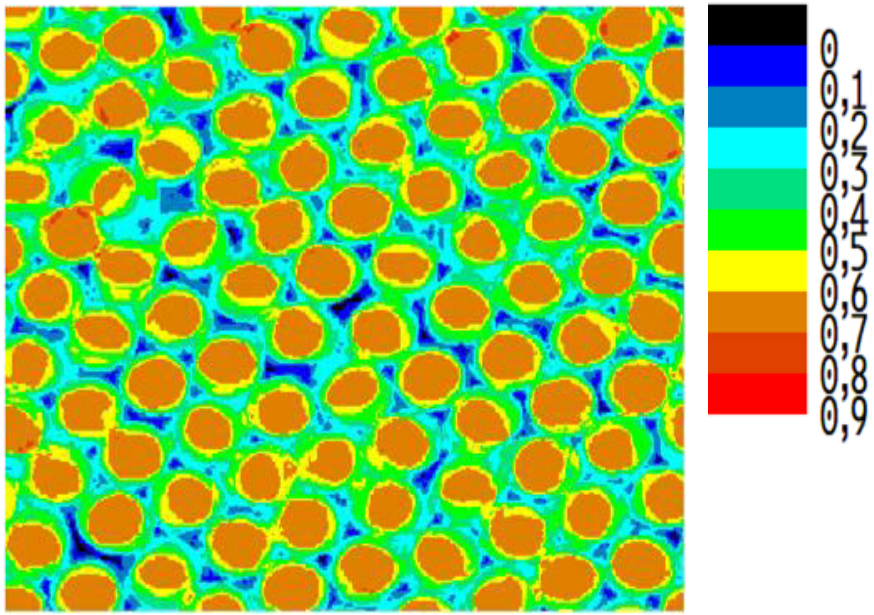


Order parameter and density distributions. Low energies

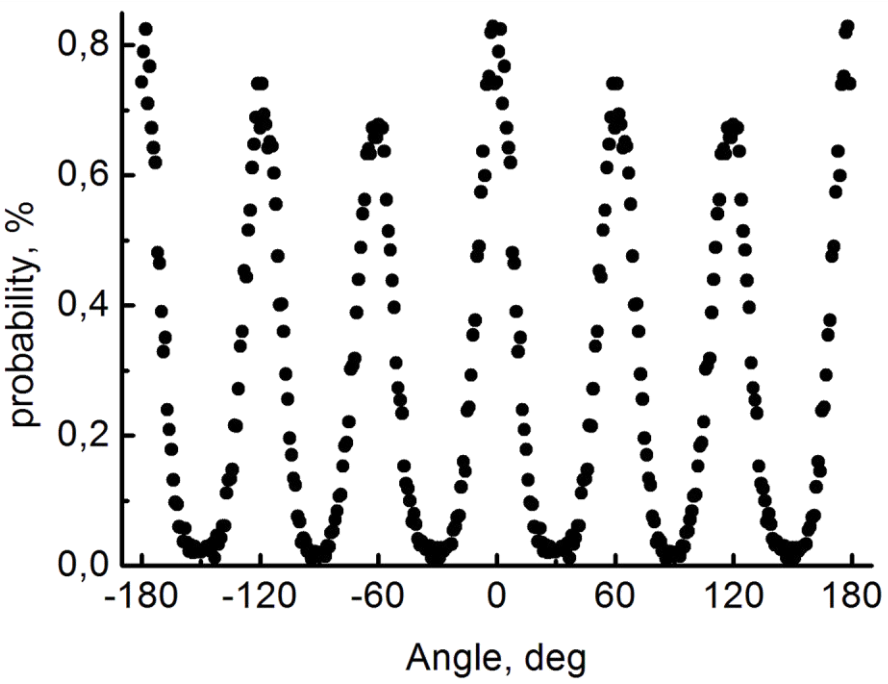
Orientation



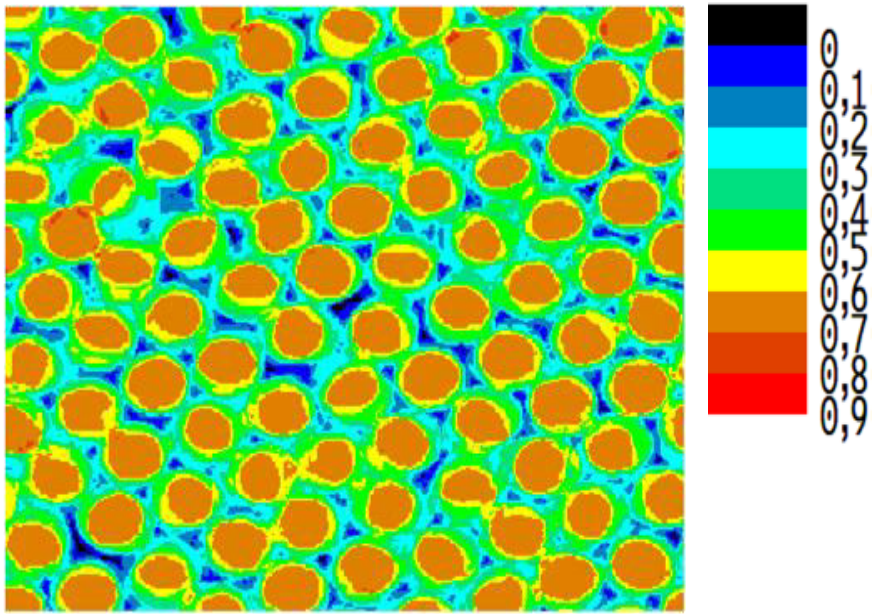
Density



Order parameter and density distributions. Low energies

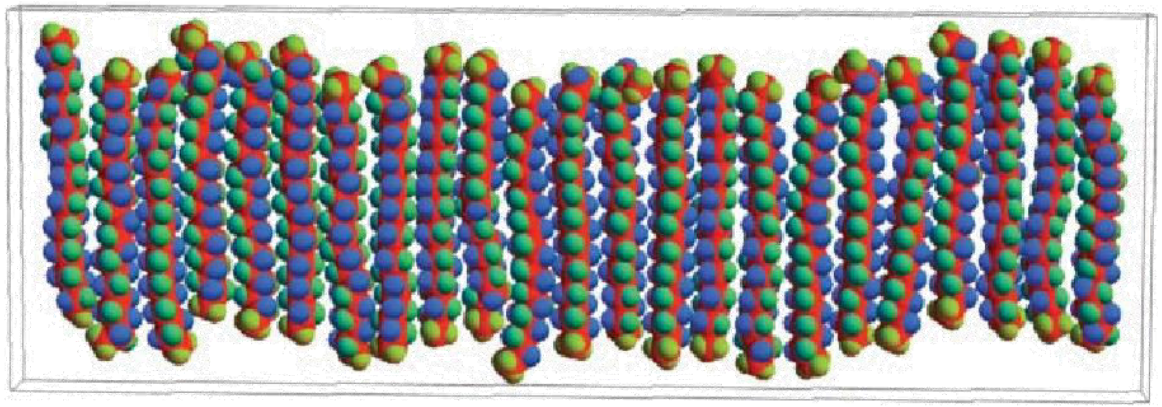


Density

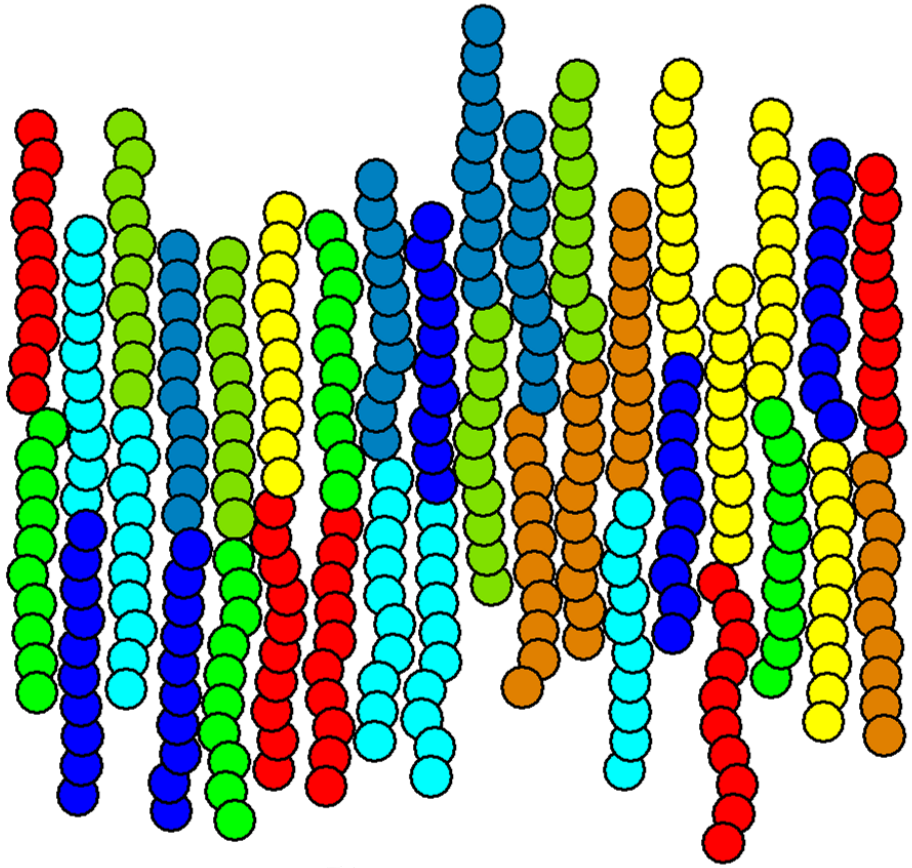


Rotator-like phase

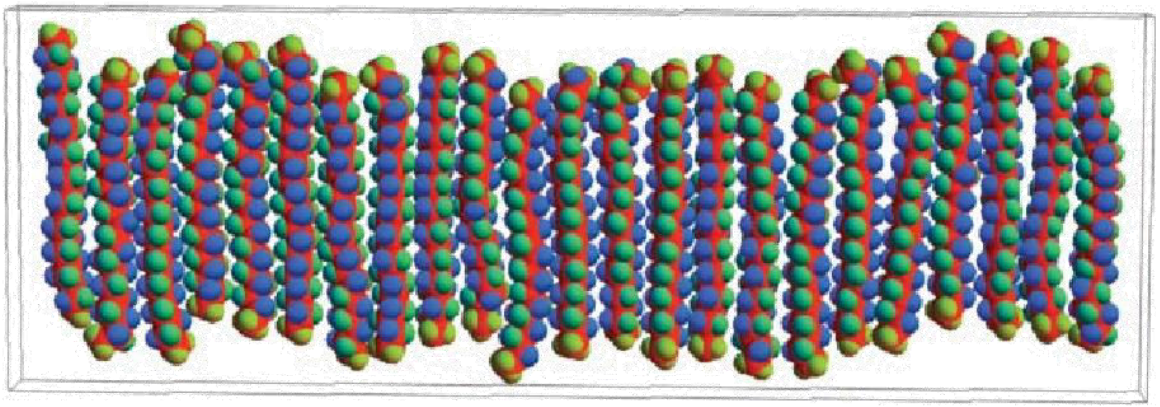
Rotator II phase



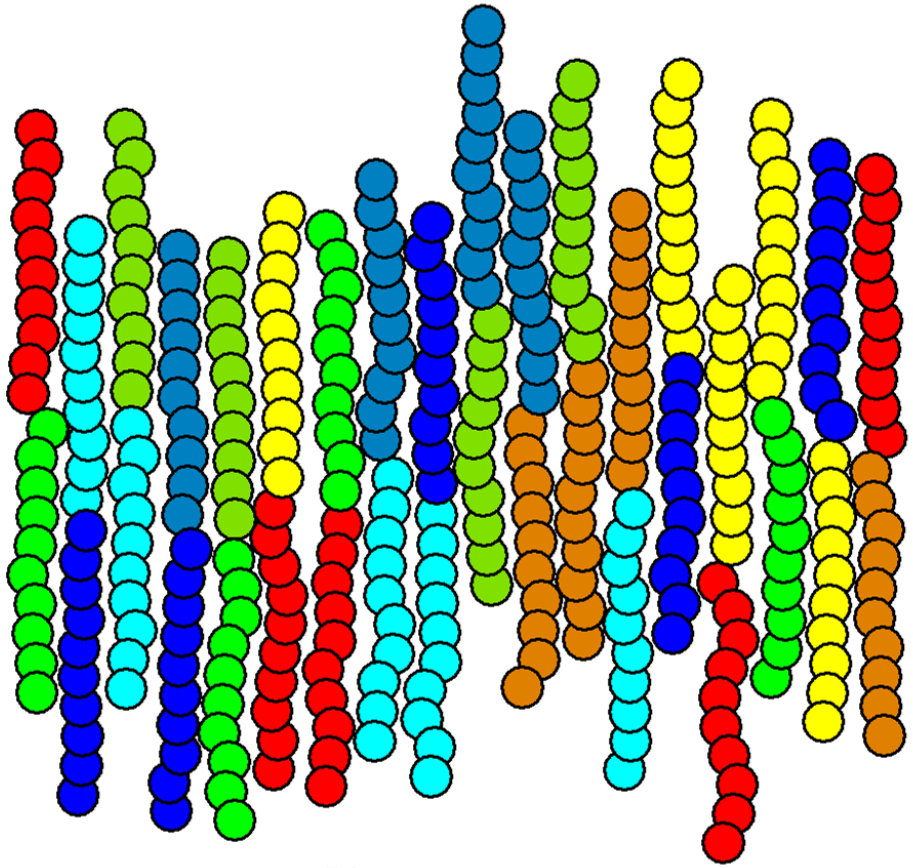
Rotator-like phase

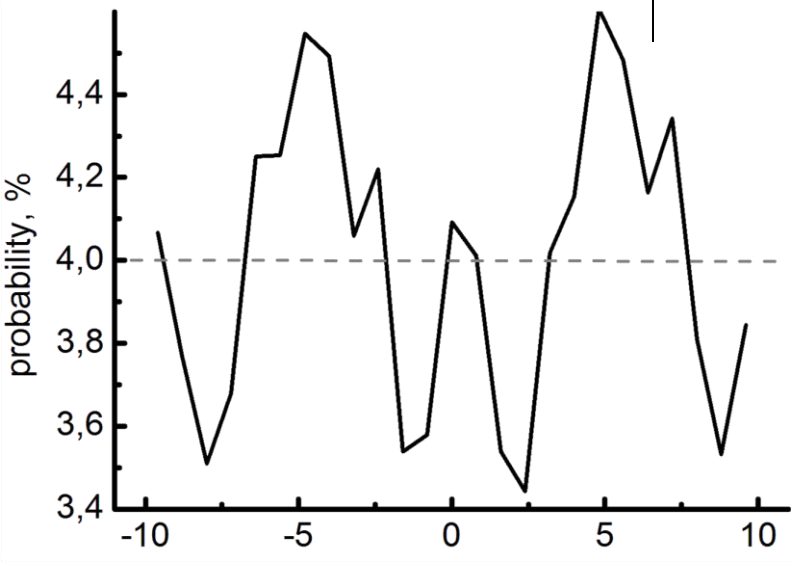


Rotator II phase

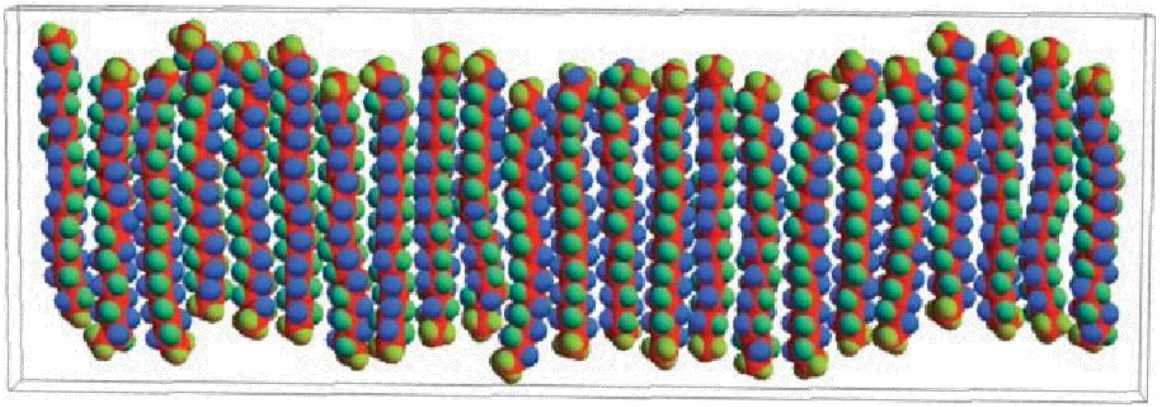


Rotator-like phase

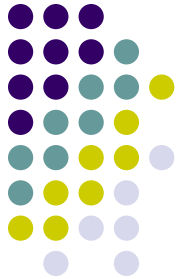




Rotator II phase

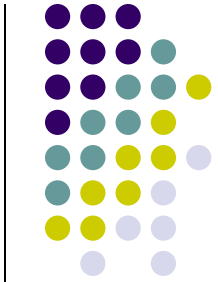


Conclusion



- System of stiff hard-sphere polymers has rotator-like phase

- WL is usable for simulations of phase transitions of polymer melts at thermodynamically equilibrium



Thank you for your attention!