Entropies of Hard Ellipse Lattices

Susanne Wagner[1], Andrij Baumketner[2], Gerhard Kahl[1]

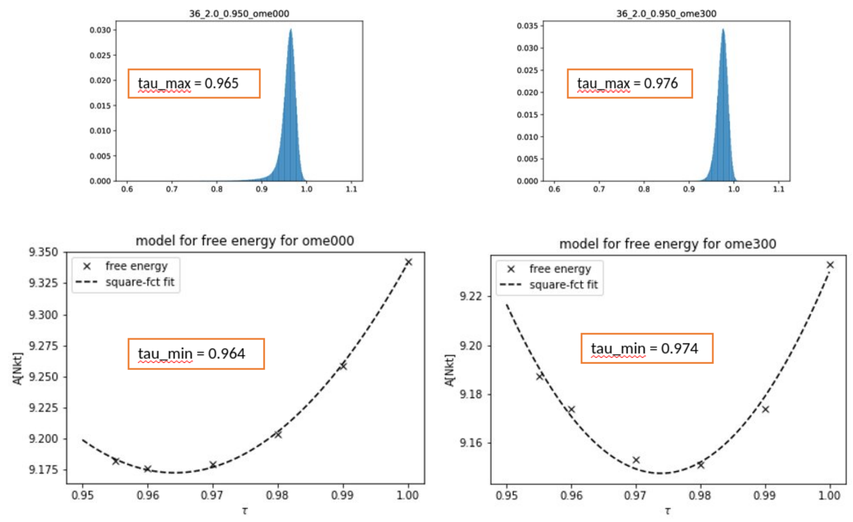
[1] ITP, TU Wien, [2] Lviv Institute of Physics and Mechanics

Introduction

- similarly to competing hcp- and fcc- hard sphere packings [1] there is an **entropic competition** between different packings of ellipses in two dimensions
- continuum of **close-packed ellipse configurations** in 2D from which only two appear to be stable → **parallel** and **diagonal** configuration.
- What is the **entropy difference** between parallel and diagonal state?

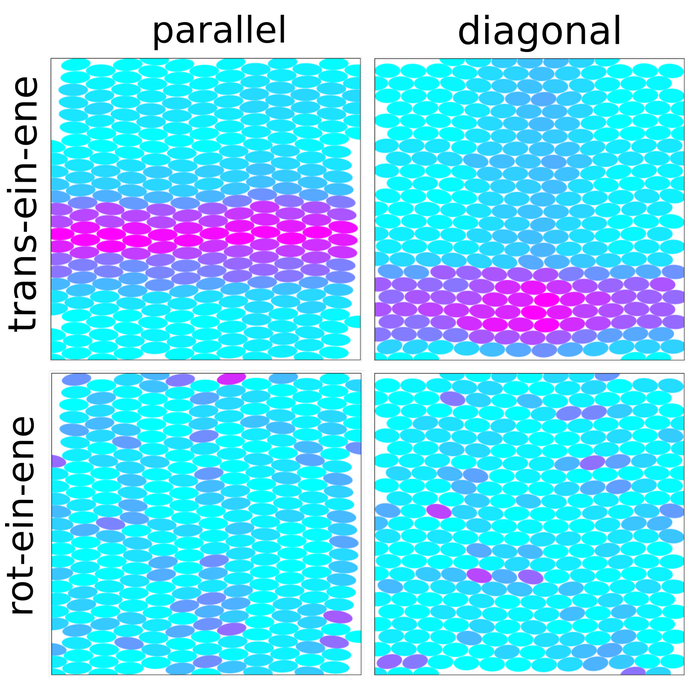
Lattice Parameterization

- a parameterization (ω, τ) was found for spanning all possible ellipse lattices
- parameter ω defines orientational and τ postional order.
- $\omega = 0$ (diagonal) and $\omega = \frac{\pi}{6}$ (parallel) are most stable states [using ω-lattice-switch]
- each $(\omega, \rho^\star)$-pair defines an optimal τ [determined using τ-lattice-switch]



Lattice Dynamics in EMM

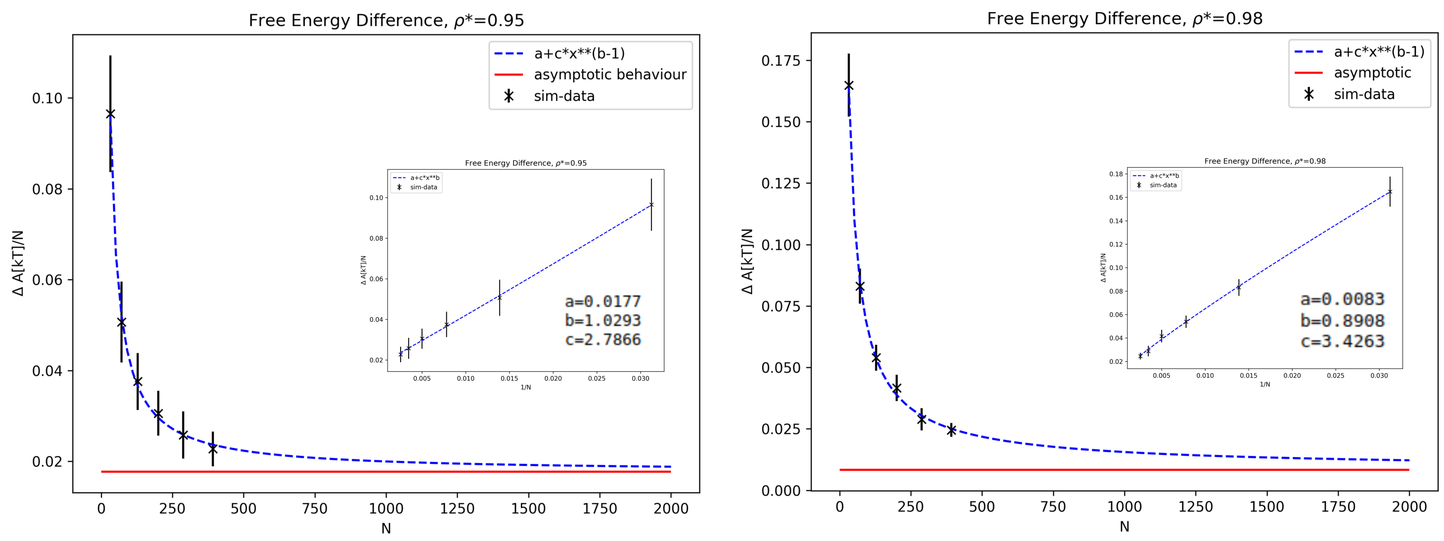
- EMM-dynamics at low spring constant for parallel and diagonal lattice (videos available!)
- translational ($\propto d\vec{u}^2$) and rotational ($\propto d\vec{\phi}^2$) Einstein Energy used for coloring scheme



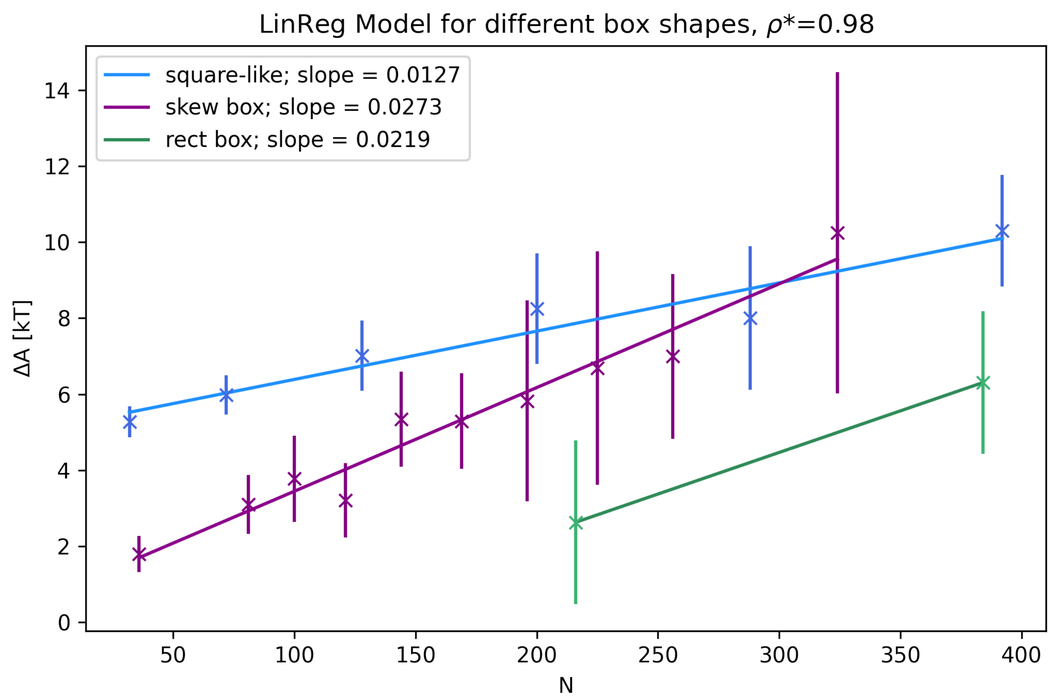
Finite Size Scaling

- **Einstein Molecule Method** [2] is applied to compute entropy-difference
- a **cascade of boxes with same geometry but different sizes** is considered for finite-size study.
- we assume a size-scaling behaviour according to [4][5]: $A_l(N) = a_l \cdot N + c_l \cdot \frac{N^b}{\kappa_l^{box}}$, with $b < 1$ and l=d,p.
- hence the **fitting model** for the free energy difference is:

$$\Delta A_{p-d}(N) = (a_p - a_d) \cdot N + (c'_p - c'_d) \cdot N^b$$



- Supported by an almost linear exponent b, we apply a linear regression model to determine the free energy difference in the thermodynamic limit from the slope of the fitted model.
- different box geometries are studied for elimiation of geometric effects:



Simulation Details

- **NVT - lattice switch Monte-Carlo** simulations searching for stable lattices within parameter space (ω, τ).
- **EMM (Einstein Molecule Method)** [2]: numeric integration from an Einstein Crystal to the Ellipse Lattice via 100 sampling points
- 1e8-2e9 cycles depending on λ-state
- mobius-transformation of integrand
- 10 independent runs for error analysis

Conclusions

- We conclude that there most certainly is a free energy difference between parallel and diagonal lattice state [3]
- At $\rho^\star = 0.98$ entropy plays in favour of the diagonal configuration.

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[3] S. Wagner, G.Kahl, A. Baumketner, to be published

[4] Bruce, Wilding, Ackland, Phys.Rev.Letters 79, 3002 (1997)âĂŃ

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Contact: **susanne.wagner@tuwien.ac.at**

Institute for Theoretical Physics, TU Wien