Monte Carlo study of alignment of microscopic disks by critical Casimir forces

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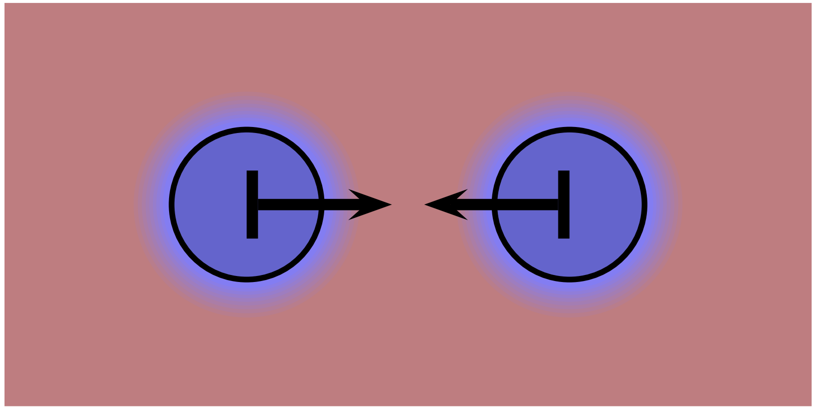
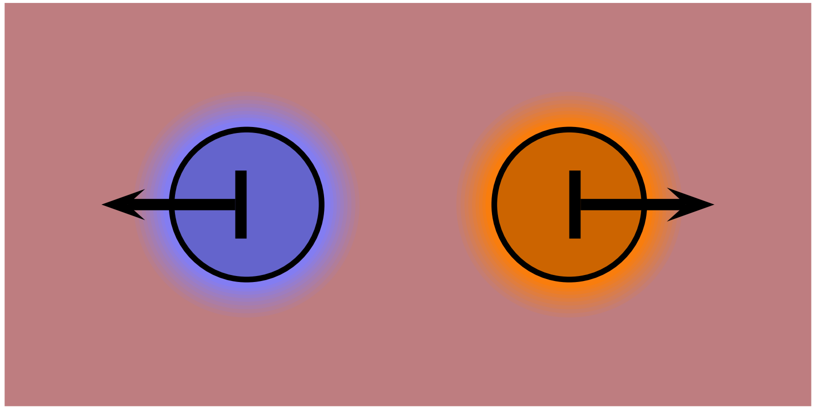
Plan

- Critical Casimir interaction
- Experiment with microscopic disks
- Potential landscape
- Monte Carlo calculation
- Results
- Conclusions

Crtical Casimir interaction

- Fluctuation-induced forces appear between objects that interact with a fluctuating medium.
- Most prominent example: Casimir force between conductors due to fluctuations of electromagnetic vacuum.
- Critical Casimir interactions originate from thermal fluctuations in a system close to its critical point.
- Dependence on boundary conditions, high temperature sensitivity.
- Universality of critical phenomena.





Experiment

- Binary mixture of water and 2,6-lutidine.
- Lower critical demixing point at $T_\mathrm{c} \approx 307\,\mathrm{K} \approx 34°\mathrm{C}$ and $w \approx 0.286$.
- 3D Ising model universality class.
- Bulk correlation length for $T < T_\mathrm{c}$:

$$\xi_\mathrm{b}(T) = \xi_0^+ \left| \frac{T - T_\mathrm{c}}{T_\mathrm{c}} \right|^{-\nu},$$

with $\nu \approx 0.63$ and $\xi_0^+ \approx 0.18\,\mathrm{nm}$.

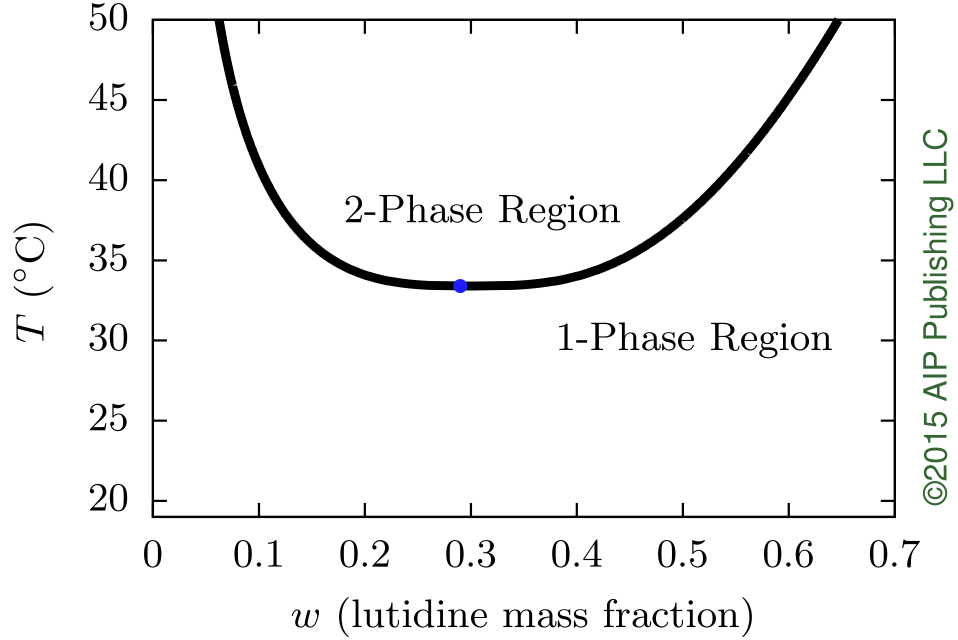
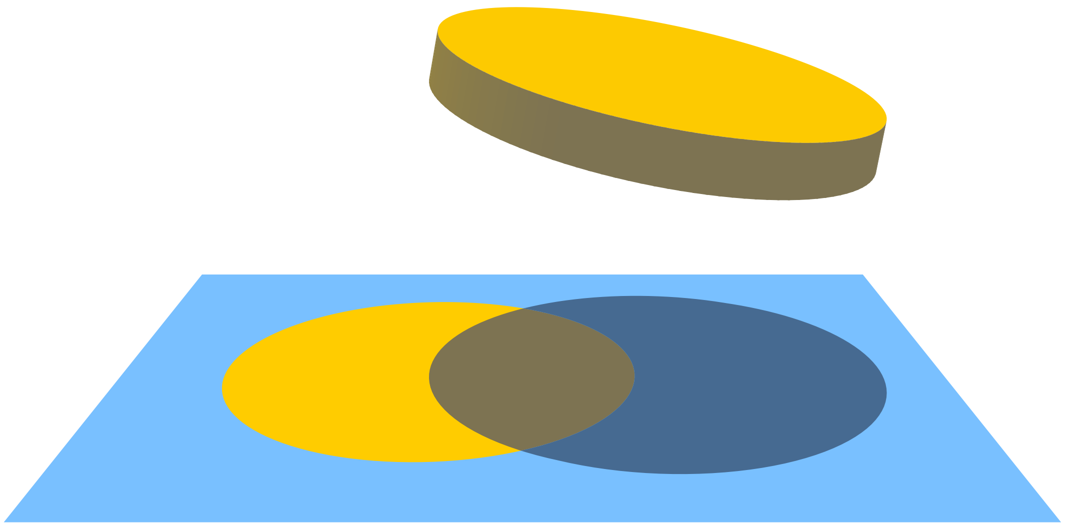
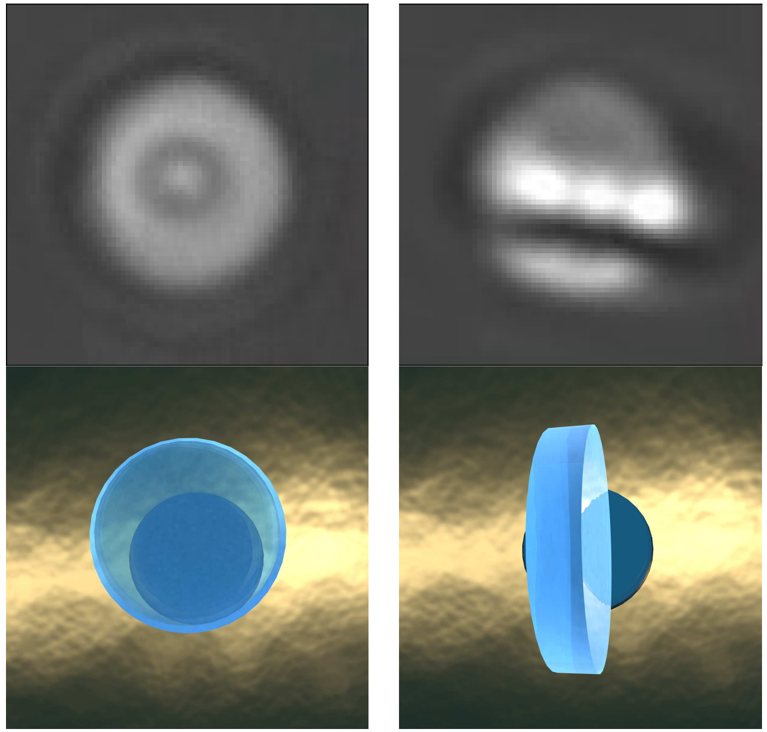


Figure adapted from *J. Chem. Phys.* **143**, 084704 (2015).

Experiment

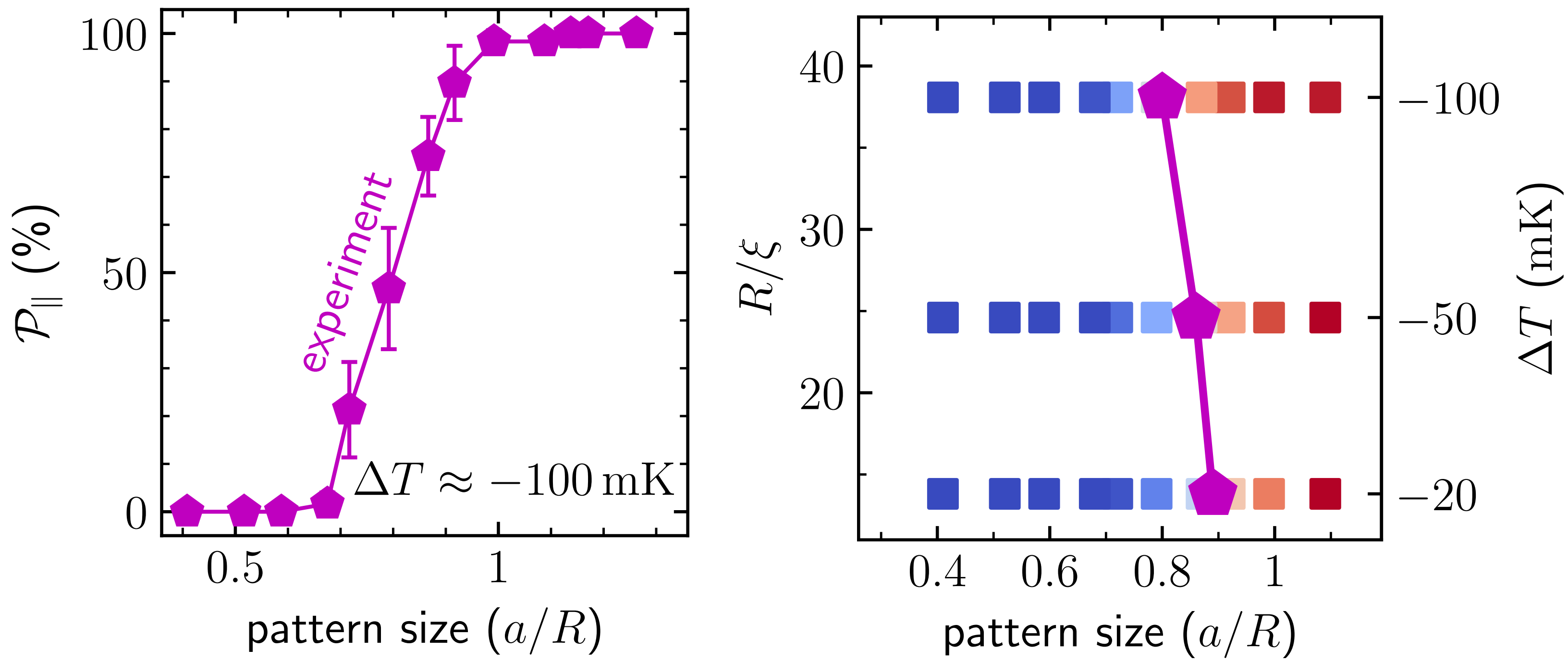
- Microscopic disk immersed in binary mixture. Diameter $2R = 2.4\,\mu\mathrm{m}$, thickness $W = 0.4\,\mu\mathrm{m}$.
- Circular patch on the flat substrate.
- Disk and patch prefer the same component of the mixture, rest of the substrate prefers the other component.
- Parallel and perpendicular configuration of the disk.





Experiment

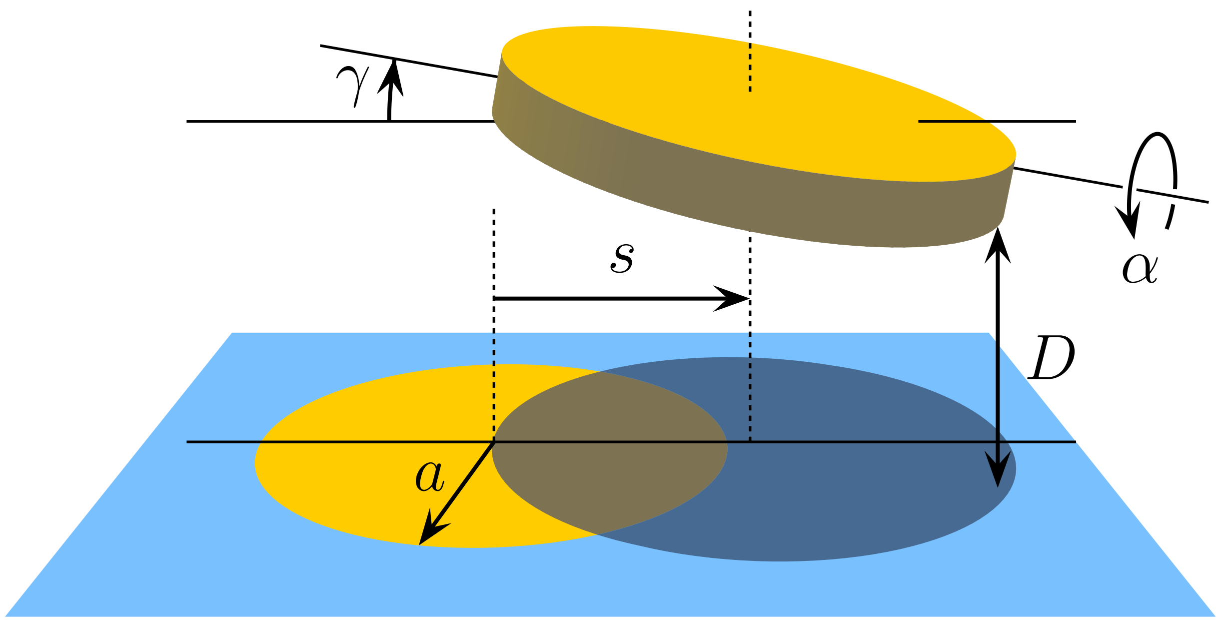
- For small patches, perpendicular configuration of the disk.
- For large patches, parallel configuration is preferred.
- Smooth crossover between two possible configurations.



$$\Delta T = T_\mathrm{c} - T$$

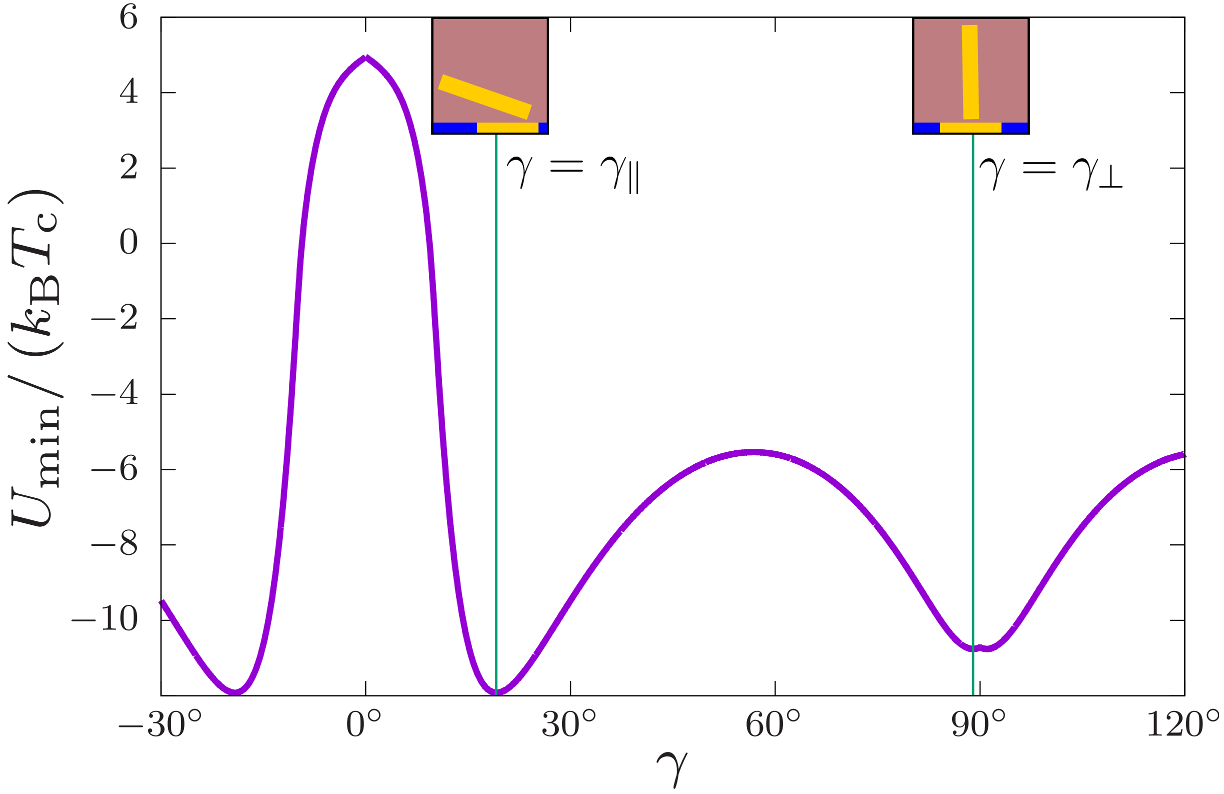
Interaction

- Interaction of the disk consists of three terms: critical Casimir, screened electrostatics, and gravity.
- Four variables describe the configuration of the particle: surface-to-surface height D, shift s, and two rotation angles α and γ.
- The interaction potential is calculated using the Derjaguin approximation.
- Rescaled variables: $\Delta = D/R$ and $\Sigma = s/R$.



Interaction

- Rich potential landscape with two local minima.
- Complicated valleys around the minima.
- Calculation of potential is too slow for a full 4D integral of Boltzmann factors.
- Monte Carlo method of estimating probabilities.



Potential U calculated for fixed $\alpha = 0°$ and various values of γ. For each set of angles, U is minimized with respect to D and s.

Monte Carlo calculation

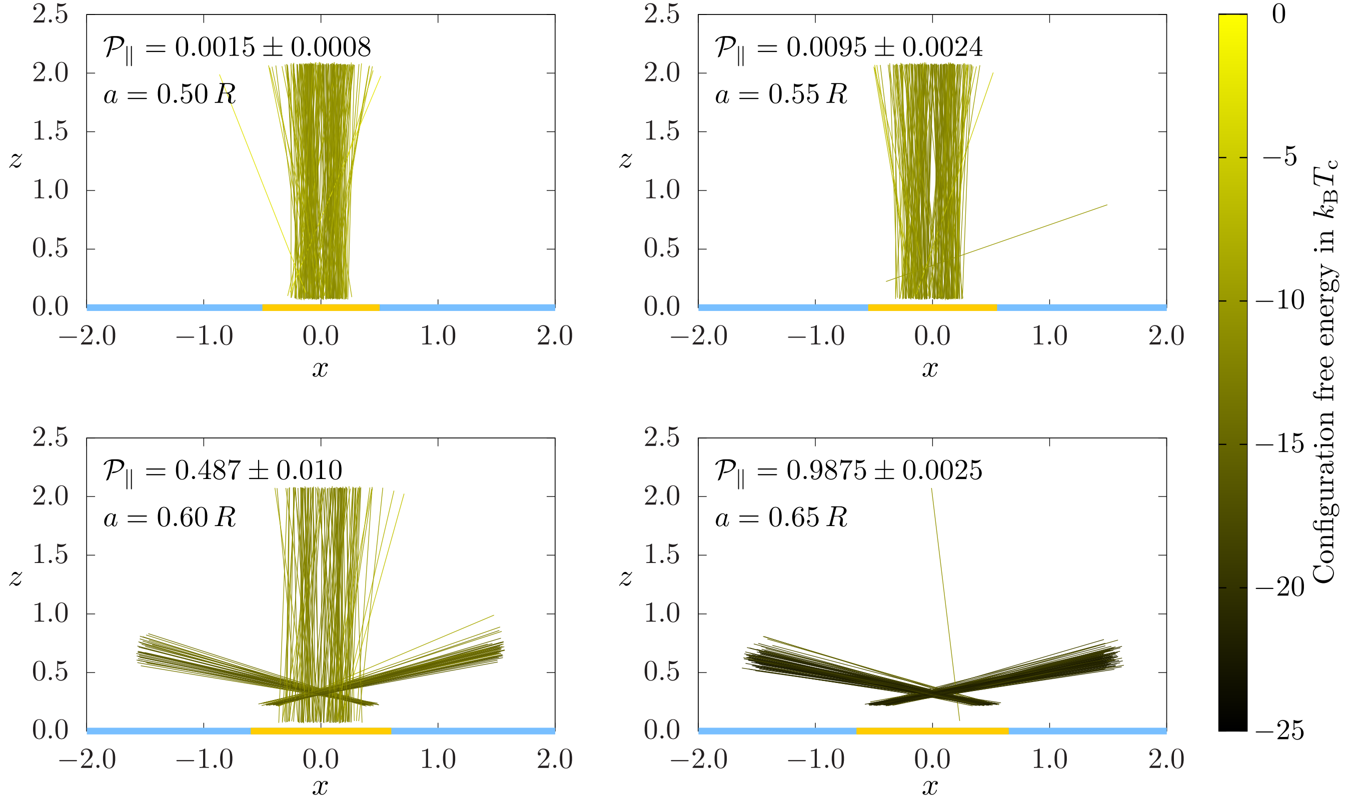
- Statistical weight of configuration of a single disk:
  $\rho\left(\Delta = D/R, \Sigma = s/R, \alpha, \gamma\right) = \left|\Sigma \cos\alpha\right| \exp\left[-U/\left(k_{\mathrm{B}} T\right)\right]$.
- Range of parameters:
  $\Delta_{\text{min}} < \Delta < \Delta_{\text{max}}, \quad -a/R < \Sigma < a/R, \quad U < U_{\mathrm{b}} + 2k_{\mathrm{B}}T$
- Initial configuration:
  random values of Δ, Σ, α, and γ with uniform distribution.
- Two types of Monte Carlo steps:

Small move	Large move
$\Delta_{\mathrm{B}} = \Delta_{\mathrm{A}} + \mathrm{rand}\left(-0.01, 0.01\right)$,	$\Delta_{\mathrm{B}} = \mathrm{rand}\left(\Delta_{\mathrm{min}}, \Delta_{\mathrm{max}}\right)$,
$\Sigma_{\mathrm{B}} = \Sigma_{\mathrm{A}} + \mathrm{rand}\left(-0.01, 0.01\right)$,	$\Sigma_{\mathrm{B}} = \mathrm{rand}\left(-a/R, a/R\right)$,
$\alpha_{\mathrm{B}} = \alpha_{\mathrm{A}} + \mathrm{rand}\left(-0.01, 0.01\right)$,	$\alpha_{\mathrm{B}} = \mathrm{rand}\left(0^\circ, 360^\circ\right)$,
$\gamma_{\mathrm{B}} = \gamma_{\mathrm{A}} + \mathrm{rand}\left(-0.01, 0.01\right)$,	$\gamma_{\mathrm{B}} = \mathrm{rand}\left(0^\circ, 360^\circ\right)$,

- Move is accepted with probability $p = \min\left(\rho_B/\rho_A, 1\right)$. If move goes outside of allowed range of variables, it is rejected.

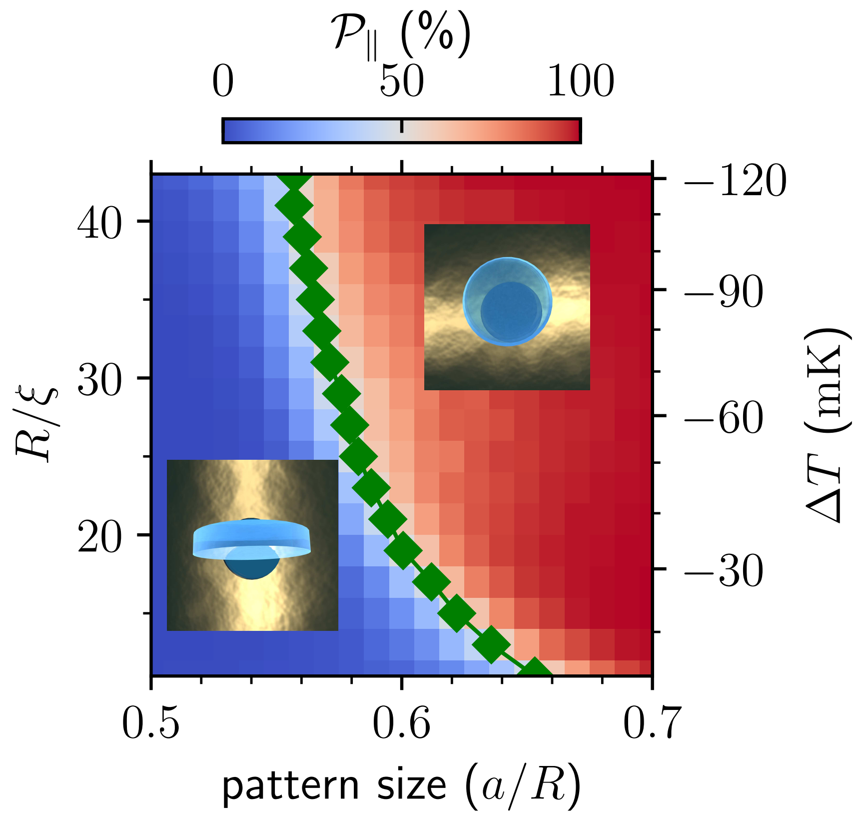
Monte Carlo calculation

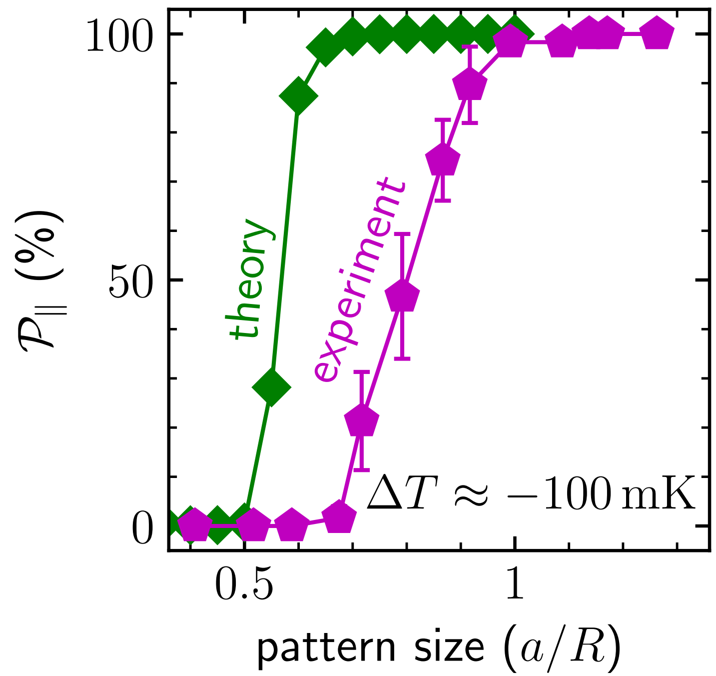
- Calculation for each particle consists of 32 small moves and 1 large move, repeated 2000 times.
- For each value of T and a/R, we do calculations for 200 independent particles.
- Classification of final disk configurations.



Results

- Results of calculations confirm the stability of the perpendicular configuration for smaller disks and the parallel configuration for larger disks.
- The location of the smooth crossover depends on the temperature.
- Qualitative agreement with experimental observations.





Conclusions

- Calculations based on the Derjaguin approximation can qualitatively explain observed parallel and perpendicular configurations of microdisk particle over circular patch.
- Monte Carlo method can be used to estimate equilibrium probabilities in canonical ensemble for complicated potential landscapes.
- Proper construction of Monte Carlo moves allows for (relatively) fast calculation.

Collaborators:
Gan Wang, Nima Farahmand Bafi, Benjamin Midtvedt, Falko Schmidt, Agnese Callegari, Ruggero Verre, Mikael Käll, **S. Dietrich**, Svyatoslav Kondrat, and **Giovanni Volpe**

Nanoalignment by critical Casimir torques, NAT. COMMUN. **15**, 5086 (2024)