# Phasenumwandlungen und Quanteneffekte in Modell-Kolloiden und Nanostrukturen

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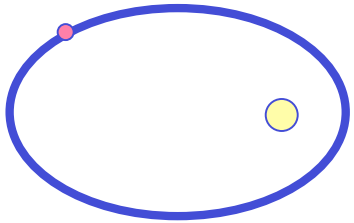
# 1 nano-meter = 1/1 000 000 000 m


**In a Europe of the size of a water droplet**
**humans have the size of a nano-meter**

# Observation/Experiment

## few particles

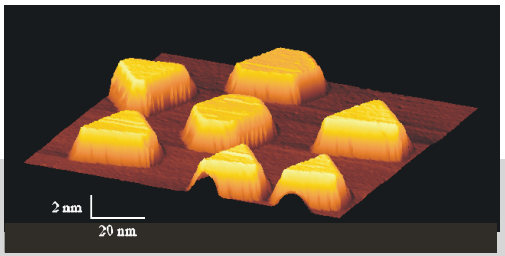
Example: solar system

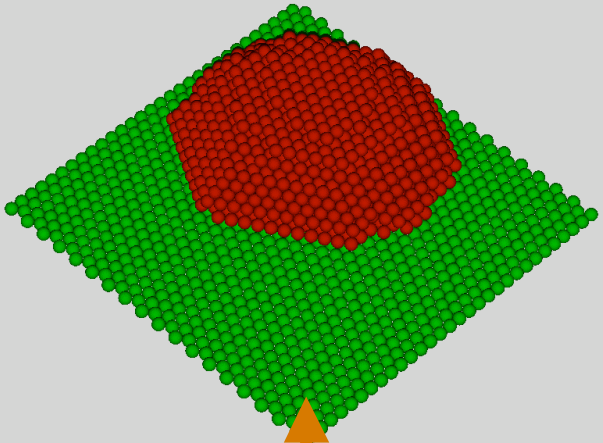


$$\phi(r) = \pm \frac{p_\phi}{m} \int_{r_0}^{r} \frac{dr}{r^2 \sqrt{\frac{2}{m}\left[E - V(r) - \frac{p_\phi^2}{2mr^2}\right]}} + \phi_0$$

Kepler-ellipses

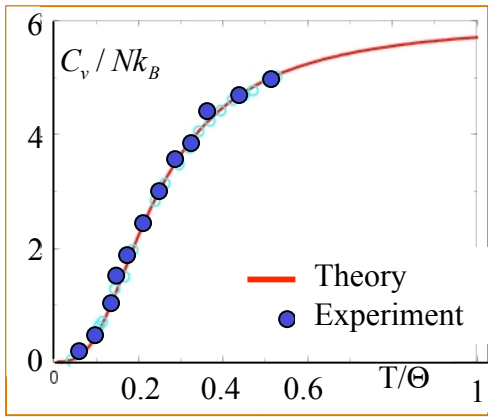
## Structures and growth at surfaces



## very many particles

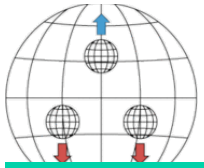
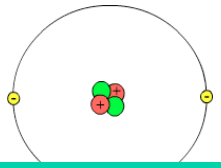
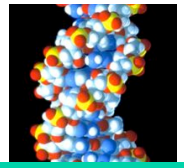
Example: heat capacity of solid




Debye-model of solids

# Simulation

# Theory



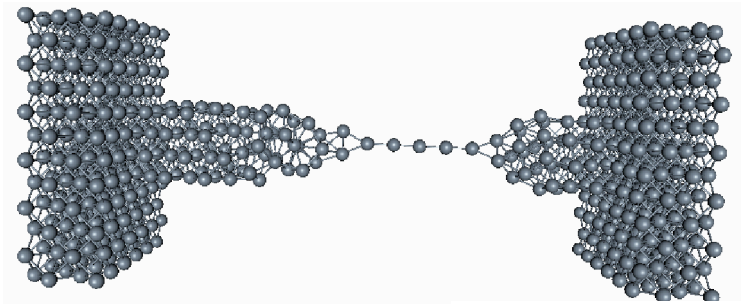
# Das Universum im Computer / LS Nielaba

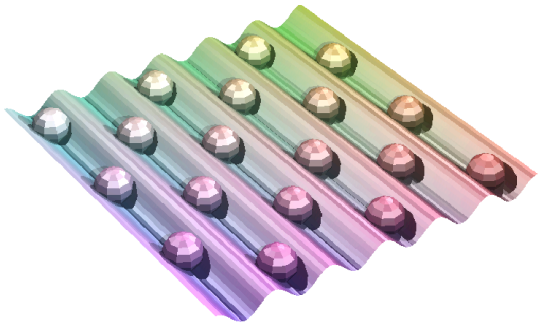
- Numerisch exakte Behandlung komplexer Systeme
- Überprüfung analytischer Näherungen
- Voraussagen fürs Experiment

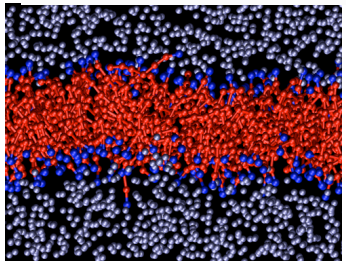
**Vielteilchensysteme** **Quantenphänomene** **Magnetismus**

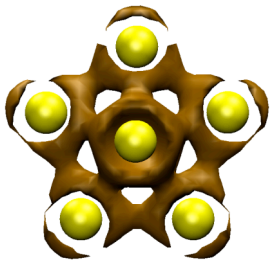
- Materialien für die Zukunft
- Struktur-Änderungen durch äußere Felder

- Nano-Bauelemente

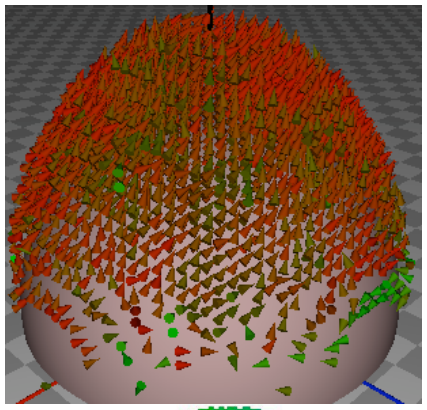


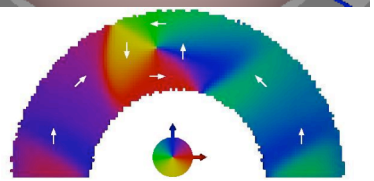






- Neue Speichermedien





*Nachbarwissenschaften:* Mathematik (Modellbildung, Methoden), Informatik, Chemie (Moleküle), Biologie (Membran), Finanz-Physik (€)

# Vortrag:

Modellkolloide: Phasenumwandlungen

Quanteneffekte

Auswirkung externer Felder

Nanostrukturen: Atomare Drähte

Cluster

Magnetische Domänen

# Mitarbeiter:

**Kolloide:**
Florian Bürzle
Kerstin Franzrahe
Peter Henseler
Marc Lohrer
Nadine Schwierz
Wolfram Strepp
K. Binder (Mainz)
A. Ricci (Mainz)
S. Sengupta (Calcutta)
D. Chaudhuri (Calcutta)

**Cluster:**
Dominik Fischer
Wolfram Quester
Margit Schach

**Drähte:**
Markus Dreher
J. Heurich (Karlsruhe)
C. Cuevas (Karlsruhe)
F. Pauly (Karlsruhe)

**Magnetische Domänen:**
Christine Schieback
Daniel Mutter
Tobias Sorg

**Experimente:** A. Erbe, C. Bechinger (Stuttgart), G. Ganteför, M. Kläui, P. Leiderer, G. Maret, U. Rüdiger, E. Scheer, K. Zahn (Konstanz)

# Methoden:

**Klassische Simulationen:**
- Monte Carlo
- Molekulardynamik
- Brownian Dynamics
- Finite Size Scaling

**Quantensimulationen:**
- Pfadintegral Monte Carlo
- Dichtefunktionaltheorie (Car-Parinello)

**Computer:**
- Großrechner (NIC, HLRS, SSC)
- lokale compute-cluster

**Kooperationen:**
- SFB TR6 (Kolloide) - “Teilsprecher” Konstanz
- SFB 767 (Nanostrukturen)
- ESF/COST (“SIMU”, “MOLSIMU”, “SIMBIOMA”) - “chairman”

**Kombinationen von Methoden zur Überbrückung von Längen-und Zeitskalen**

# Simulationen in der Statistischen Physik

Statistische Mittelwerte :

$$\langle A \rangle = \frac{1}{Z} \int d\{\mathbf{X}\} A(\mathbf{X}) \exp\left[ - H(\mathbf{X}) / k_B T \right]$$

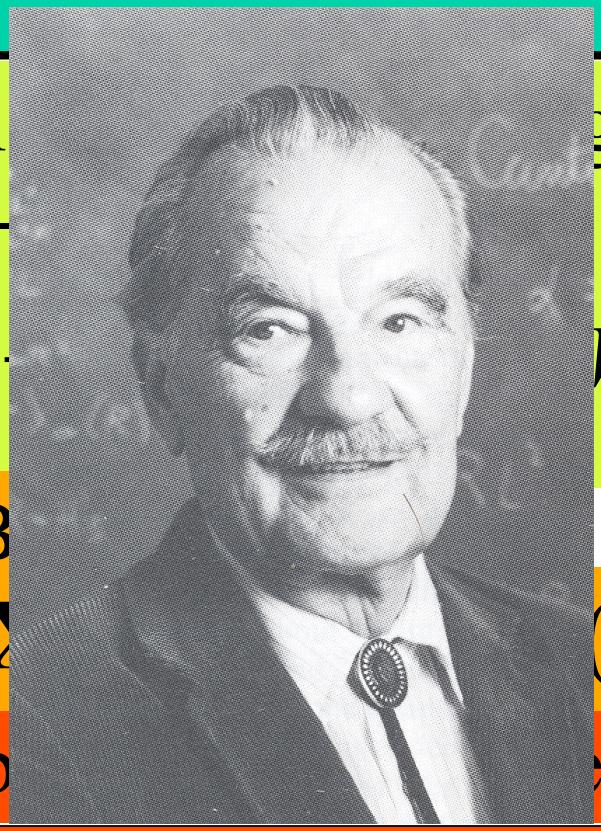
dabei: $$Z = \int d\{\mathbf{X}\} \exp\left[ - H(\mathbf{X}) / k_B T \right]$$

Im Gleichgewicht :

$$P_{eq}(\mathbf{X}) = \frac{1}{Z} \exp\left[ - H(\mathbf{X}) / k_B T \right]$$

$$\langle A \rangle = \frac{1}{M} \sum_{i=1}^{M} A(\mathbf{X}_i)$$

# Metropolis Monte Carlo:



•Wahrscheinl g im Phasenraum:

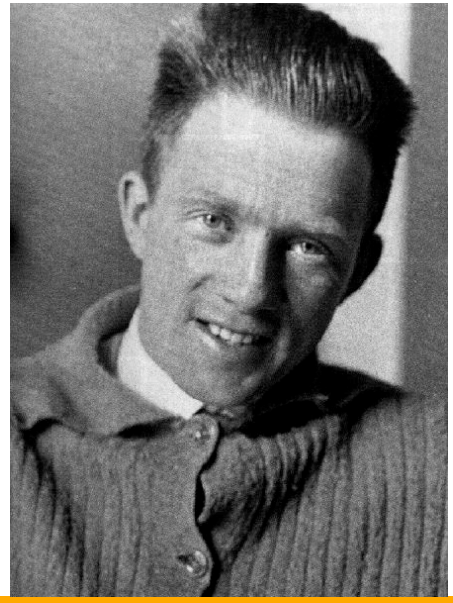
$$P(\mathbf{X},t+1) = \sum_{X'} W(\mathbf{X}' \rightarrow \mathbf{X}) P(\mathbf{X}',t) - W(\mathbf{X} \rightarrow \mathbf{X}') P(\mathbf{X},t)$$

•detaillierte B

$$W(\mathbf{X}' \rightarrow \mathbf{X}) P_{eq}(\mathbf{X}') = W(\mathbf{X} \rightarrow \mathbf{X}') P_{eq}(\mathbf{X})$$

•Wahl für Üb einlichkeiten:

$$W(\mathbf{X} \rightarrow \mathbf{X}') = \begin{cases} \exp(-\beta \Delta H[\mathbf{X} \rightarrow \mathbf{X}']) : \Delta H \geq 0 \\ 1 : \Delta H \leq 0 \end{cases}$$

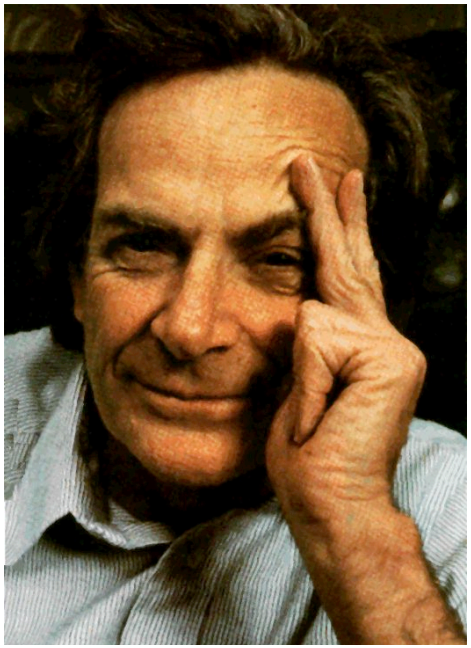


Statistische Mechanik

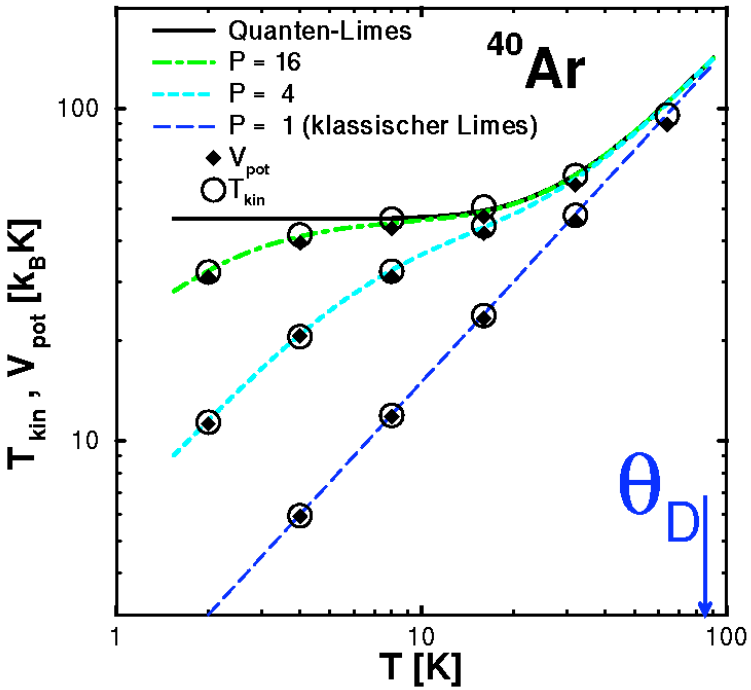
Quantenmechanik

Feynman (1942)

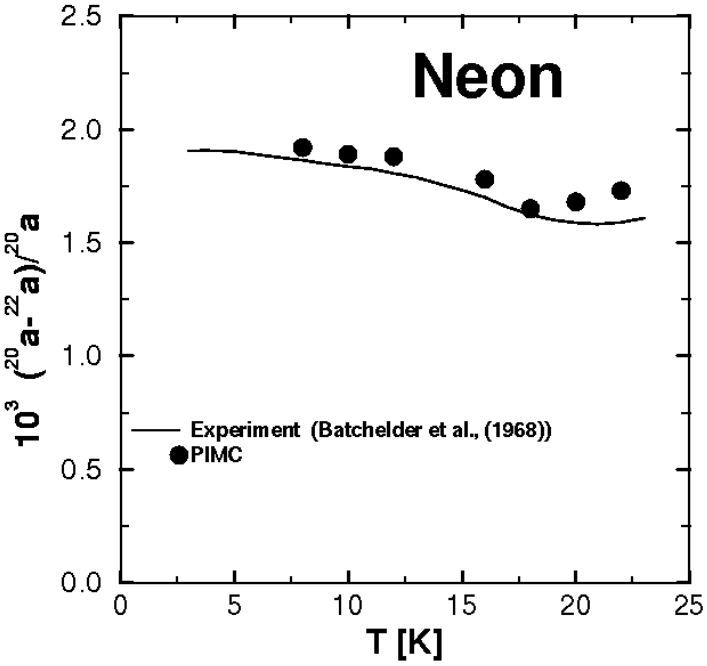
Pfadintegrale



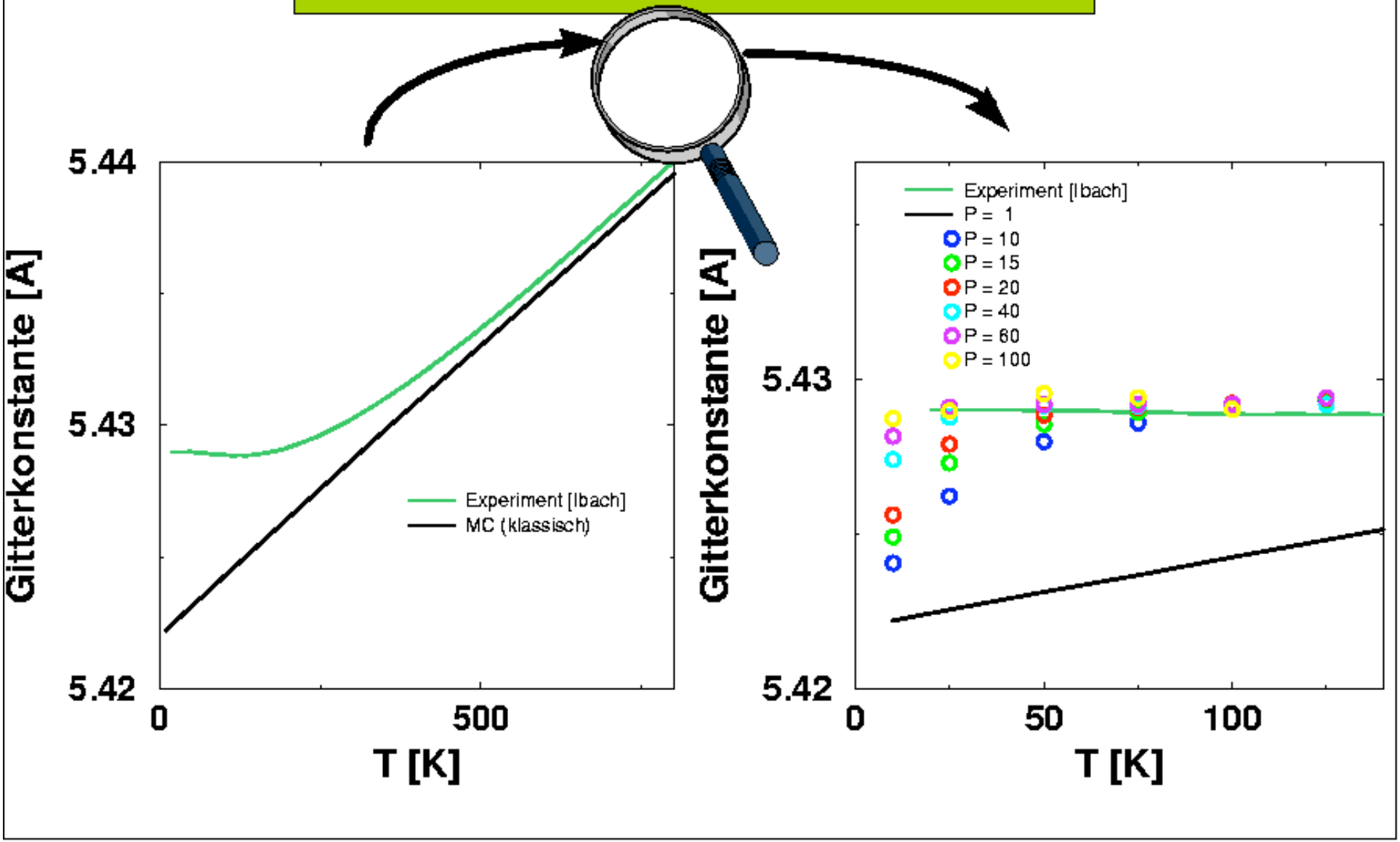
# Quanteneffekte in Festkörpern: Pfadintegral Monte Carlo Studien

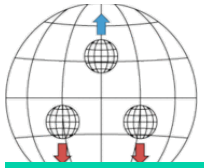
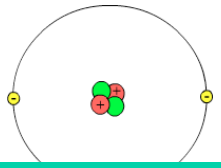
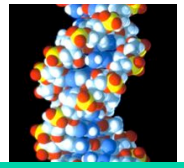



| Element | Debye-Temperatur $\theta_D$[K] |
|---|---|
| Ar | 85 |
| Al | 394 |
| Li | 400 |
| Si | 625 |
| Ge | 360 |
| Cu | 315 |
| Fe | 420 |



# Volumen in Si- Festkörpern





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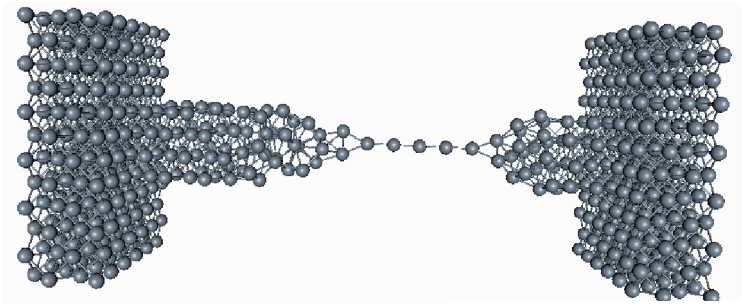

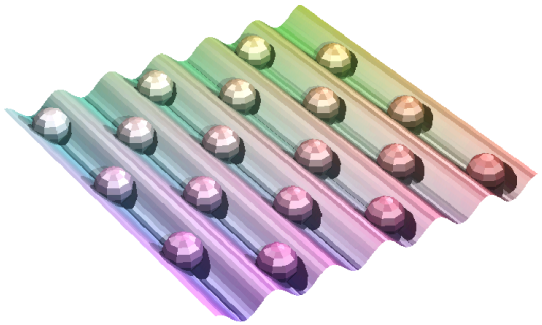

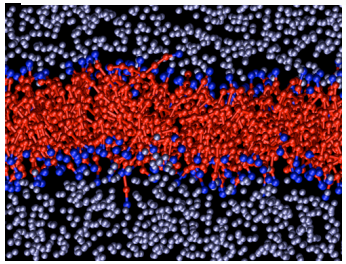

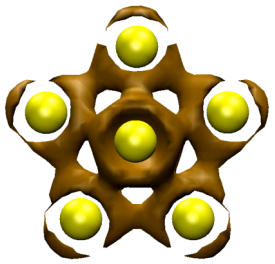

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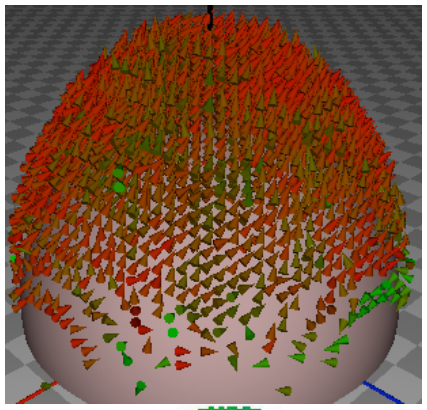

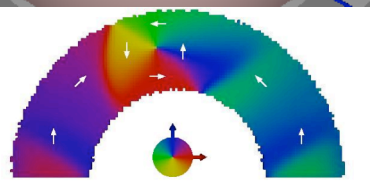

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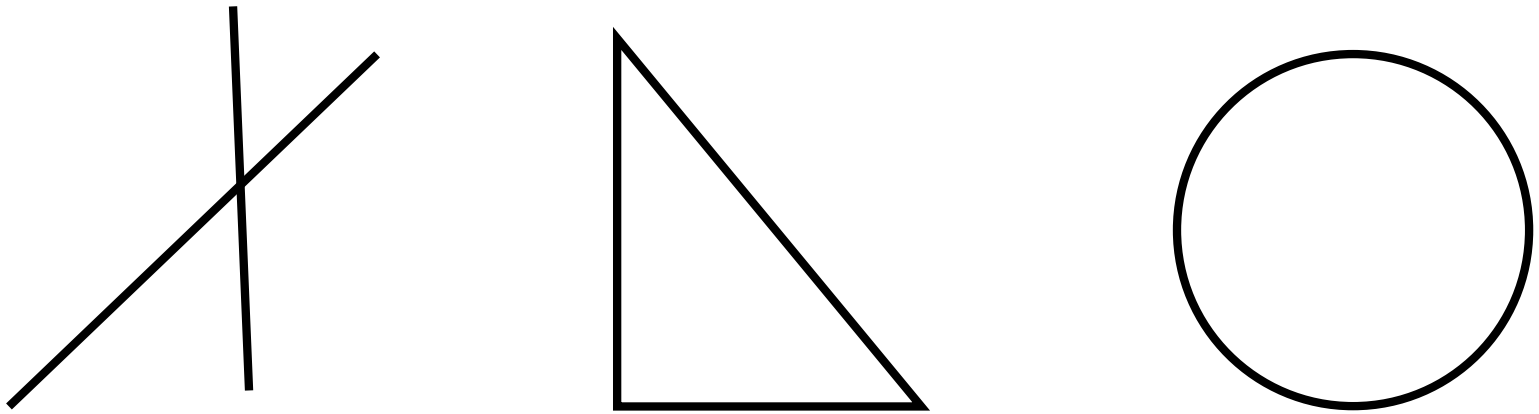
# Einfache geometrische Objekte:



# Colloidal dispersions:

Solutions of mesoscopic solid particles with a stable (non-fluctuating) shape embedded in a molecular fluid solvent

Examples: aqueous suspensions of polystyrene,
latex spheres or rods,…

They can be prepared and characterized in a controlled way

The interaction is tunable

They are prototypes of soft matter: Simplest complex fluid

→ Ideal model systems in statistical physics

→ "Bridge" to the Nano-World

# Colloidal dispersions:

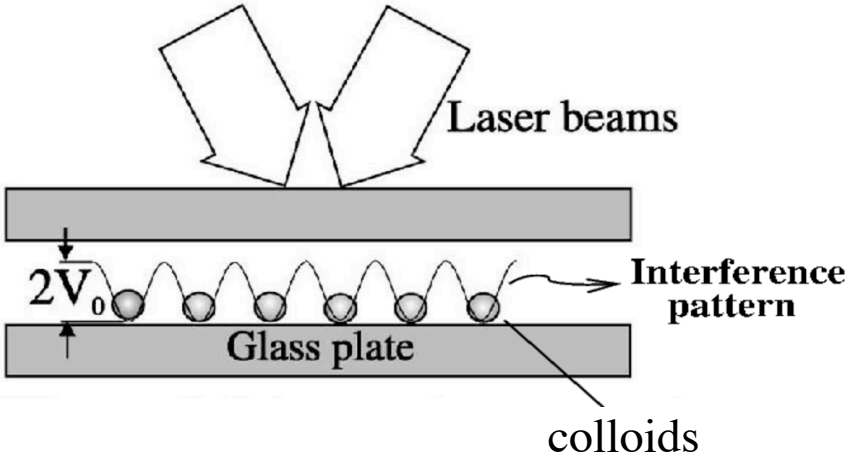
Strukturen im Gleichgewicht:
Phasenumwandlungen und Quanteneffekte

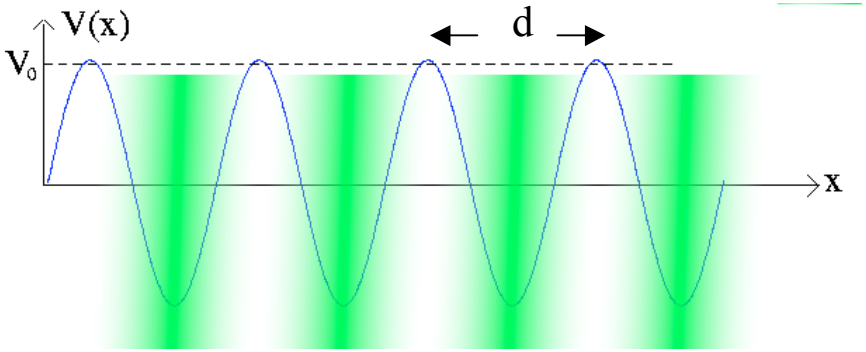
Strukturbildung im Nichtgleichgewicht

Vergleich mit Experimenten und Voraussagen

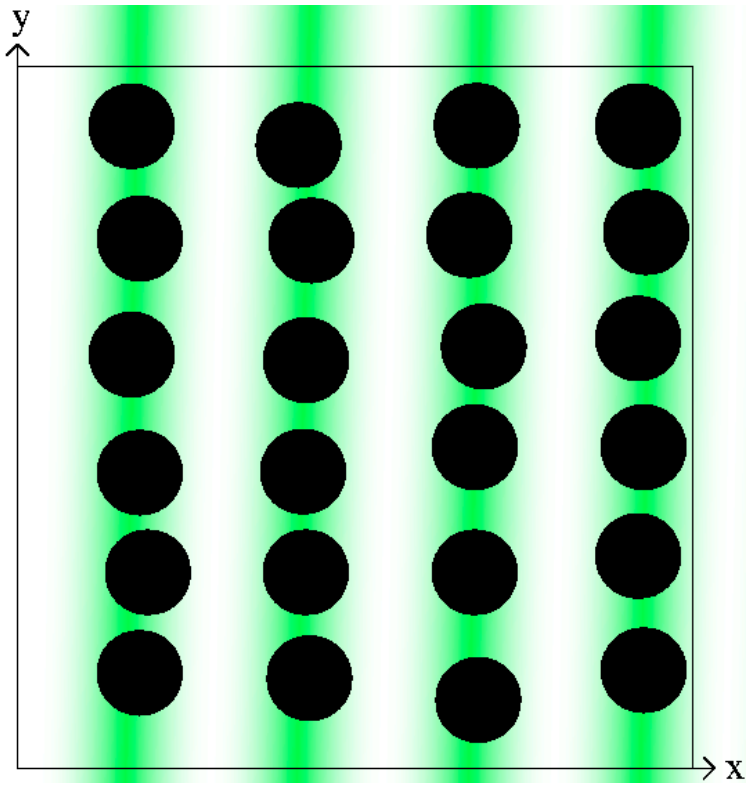
# Colloids in external periodic light fields (experiments):

Side view:



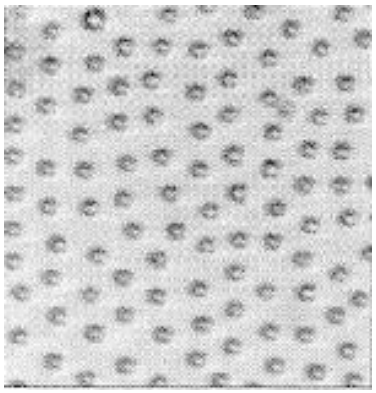
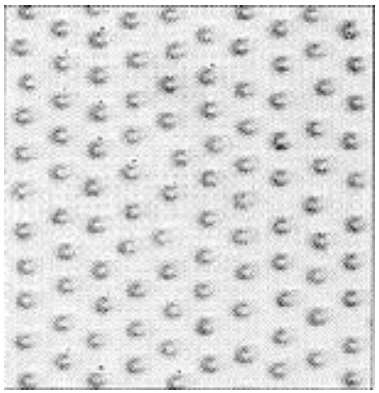
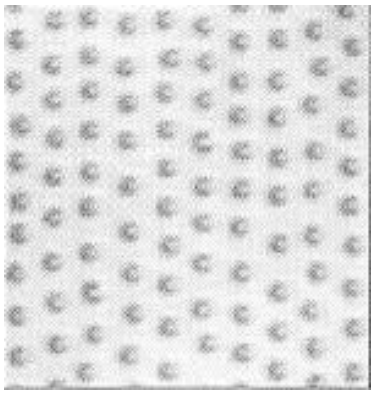
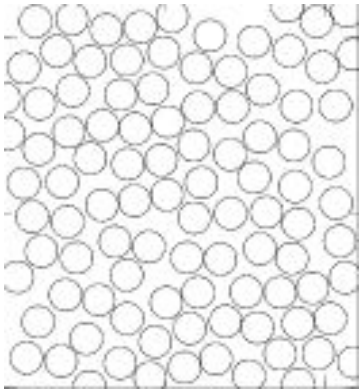
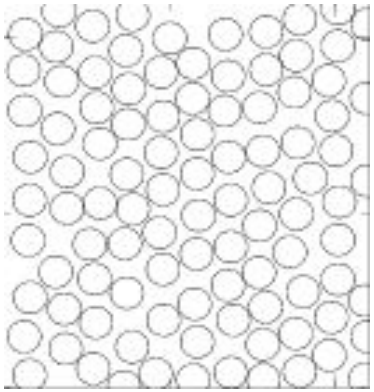
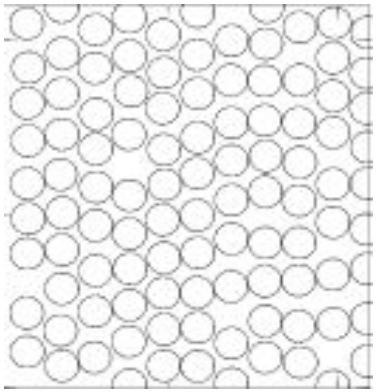

Top view:




Q.-H. Wei, C. Bechinger, D. Rudhardt, P. Leiderer, Phys. Rev. Lett. **81**, 2606 (1998)

# Comparison experiment/simulation

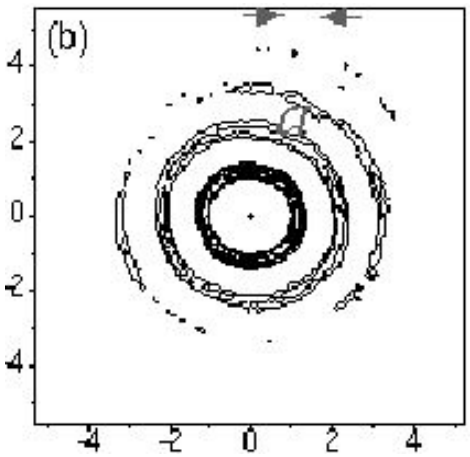
## Configurations

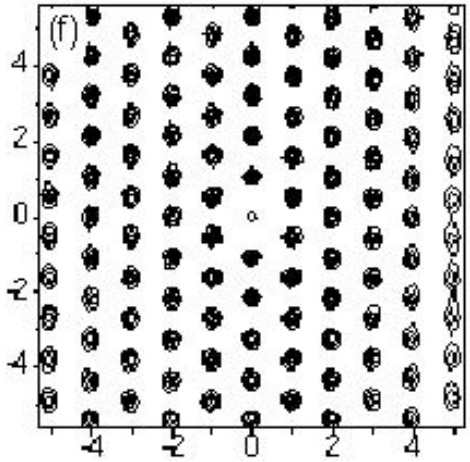







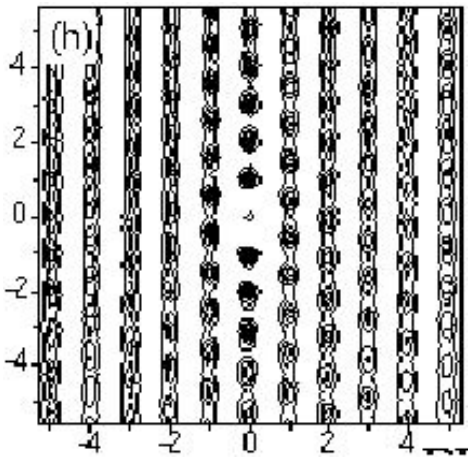
$V_0$ →

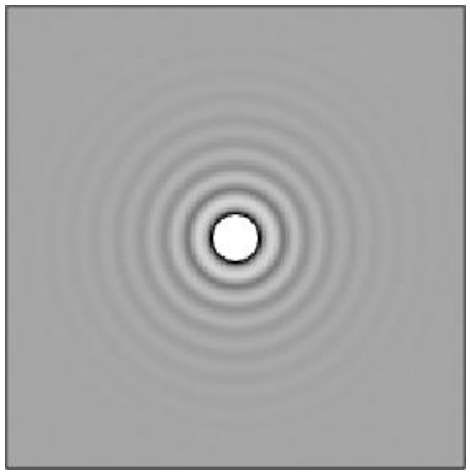
# Comparison experiment/simulation

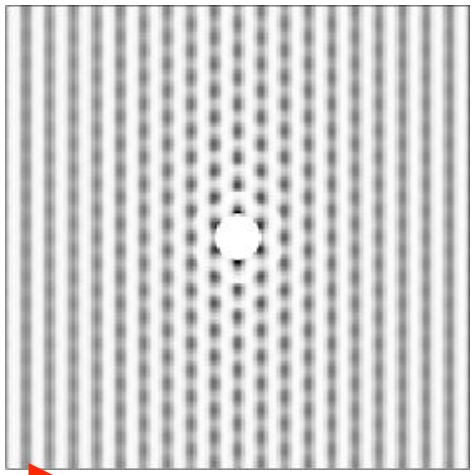
## Pair correlation functions

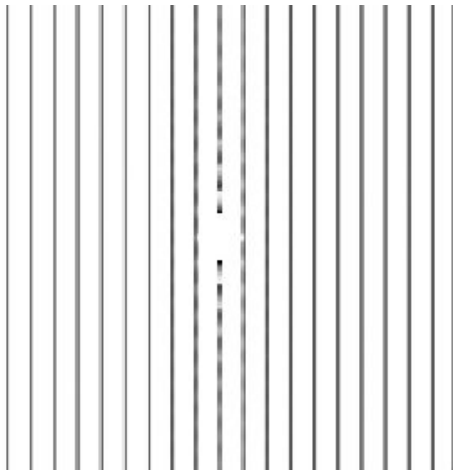






$V_0$ →

# The cumulant:

Order parameter: $\Phi$

$$U_L = 1 - \frac{\left\langle \Phi^4 \right\rangle_L}{3\left\langle \Phi^2 \right\rangle_L^2}$$

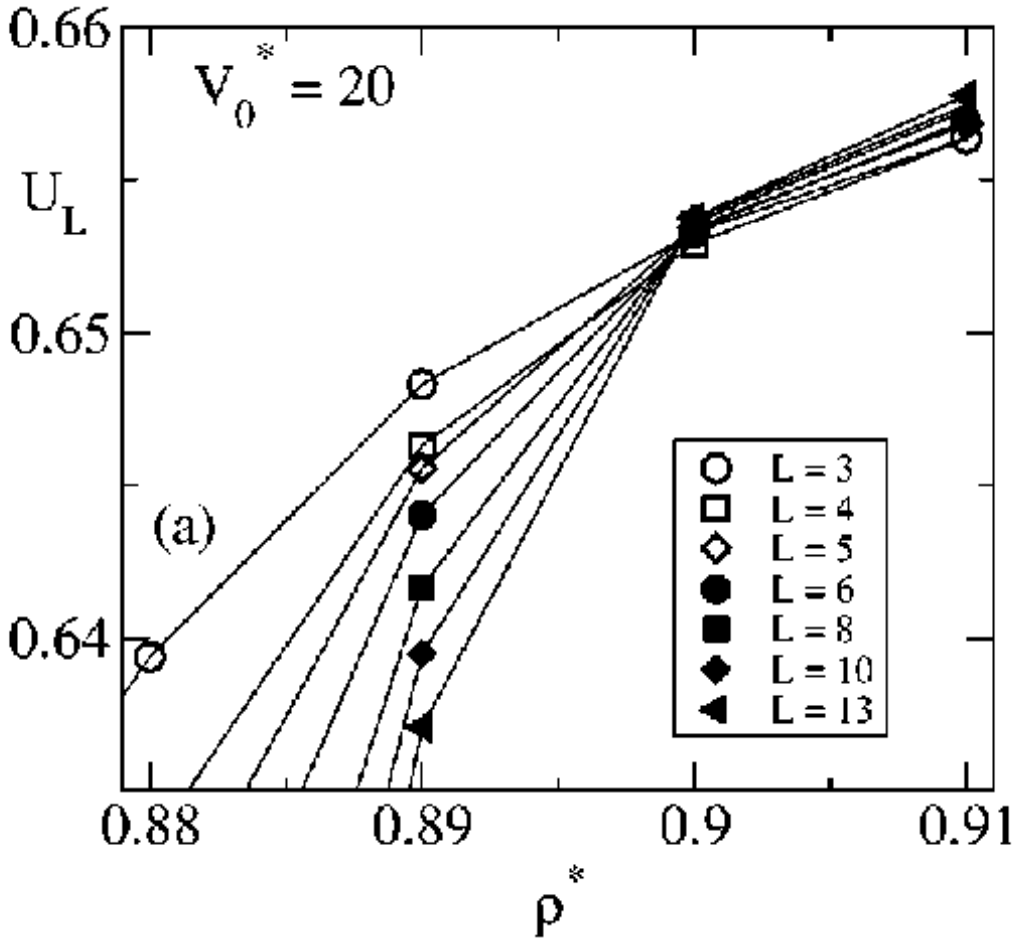
T>$T_c$: $U_L \xrightarrow{L\to\infty} 0$

T<$T_c$: $U_L \xrightarrow{L\to\infty} 2/3$

T=$T_c$: $U_L \approx U_L(L/\xi) \xrightarrow{\xi\to\infty} U^*$ (*universal*)

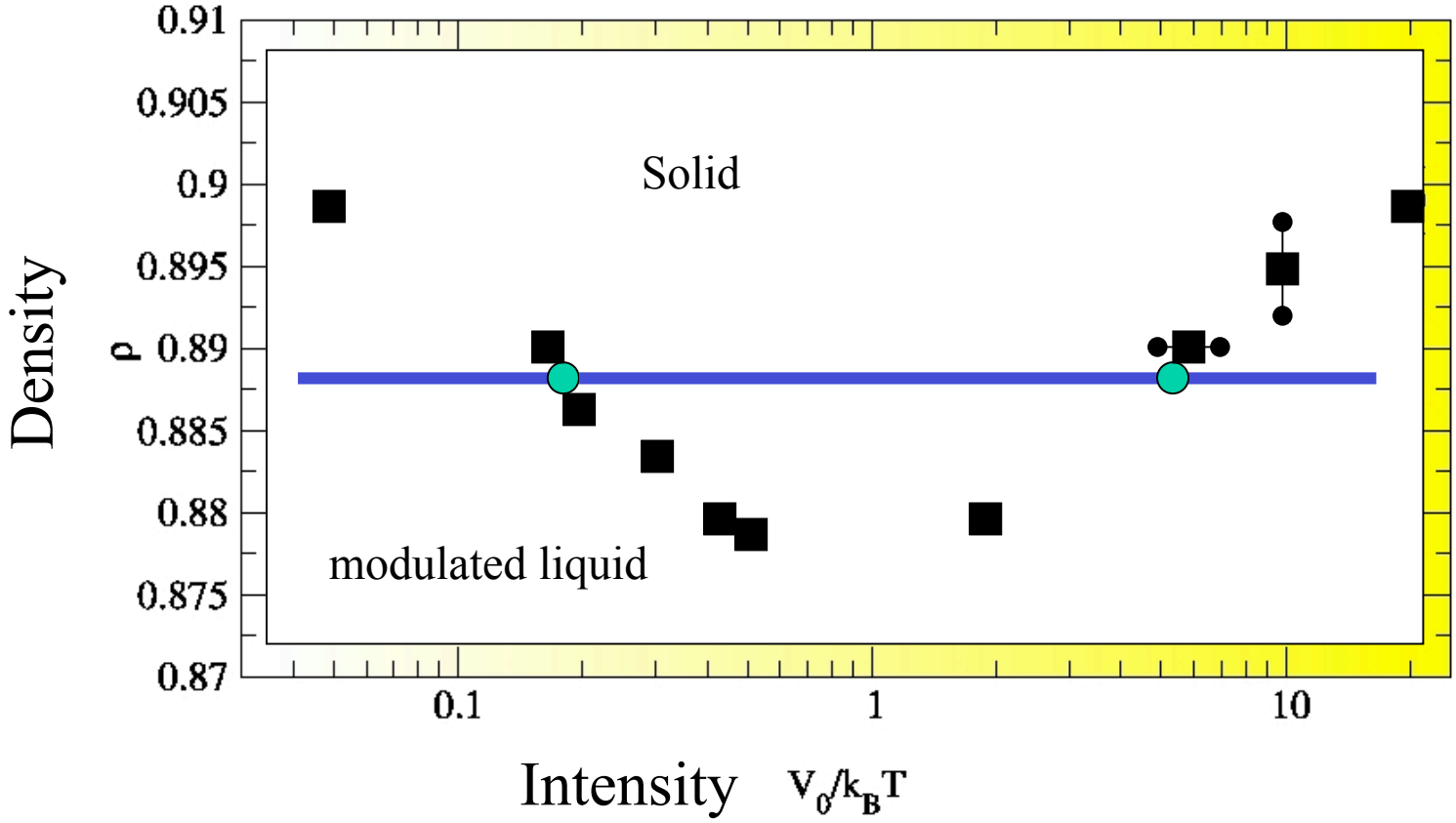
K. Binder, Z. Phys. B43, 119 (1981)

# Order parameter cumulant:

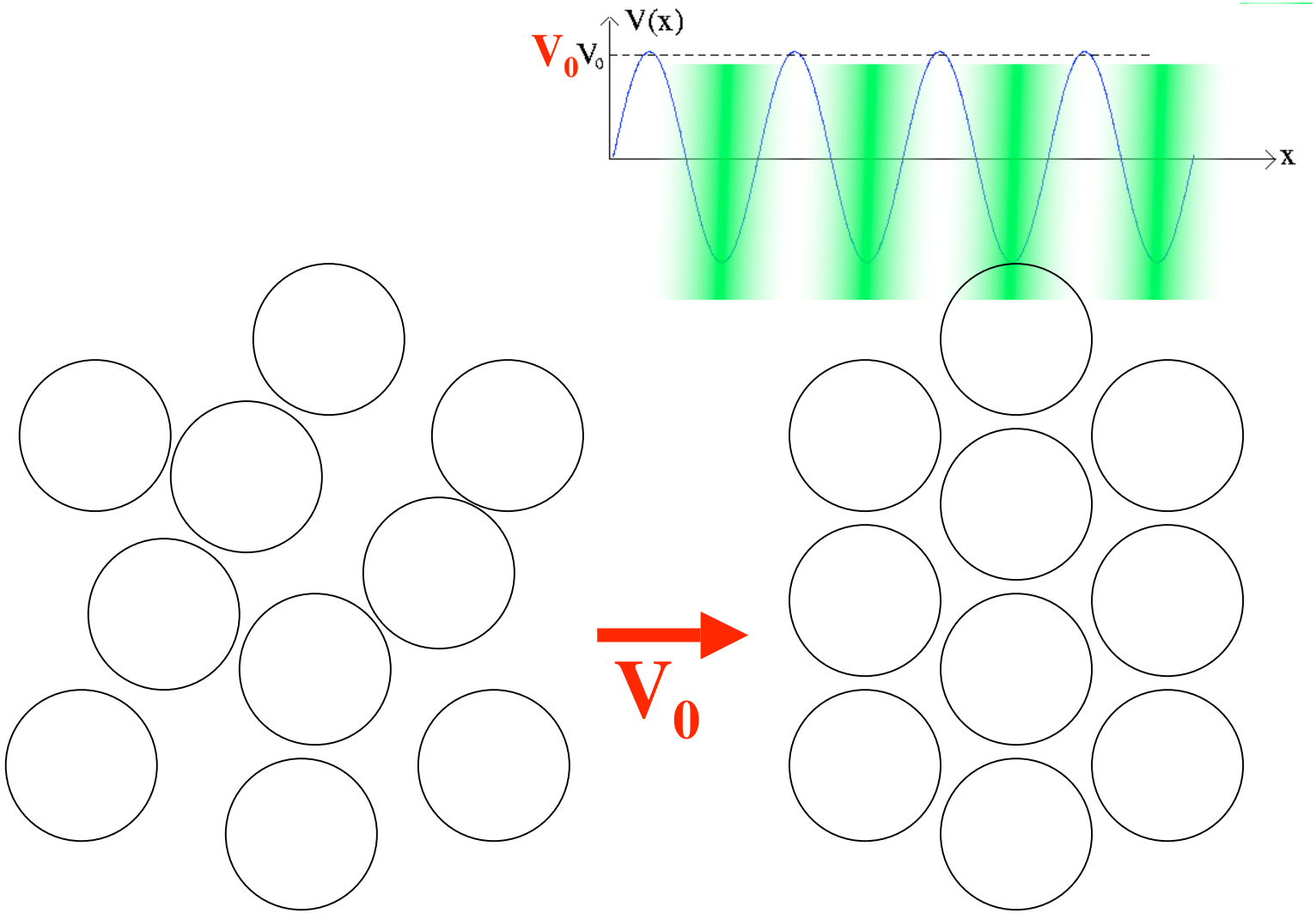



W. Strepp, S. Sengupta, P. Nielaba, PRE 63, 046106 (2001)

# Phase diagram (hard disks):

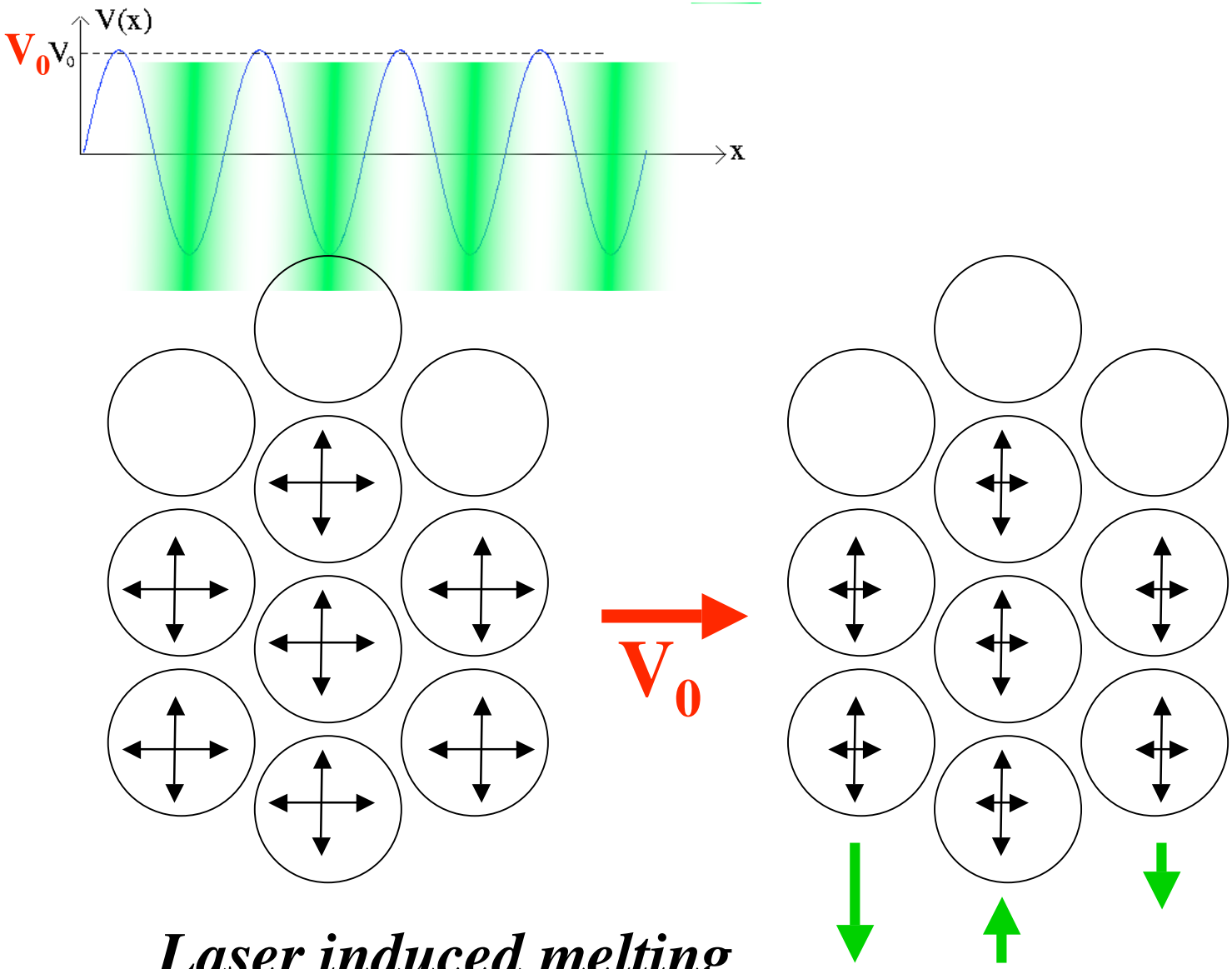


# Suppression of fluctuations for small $V_0$:



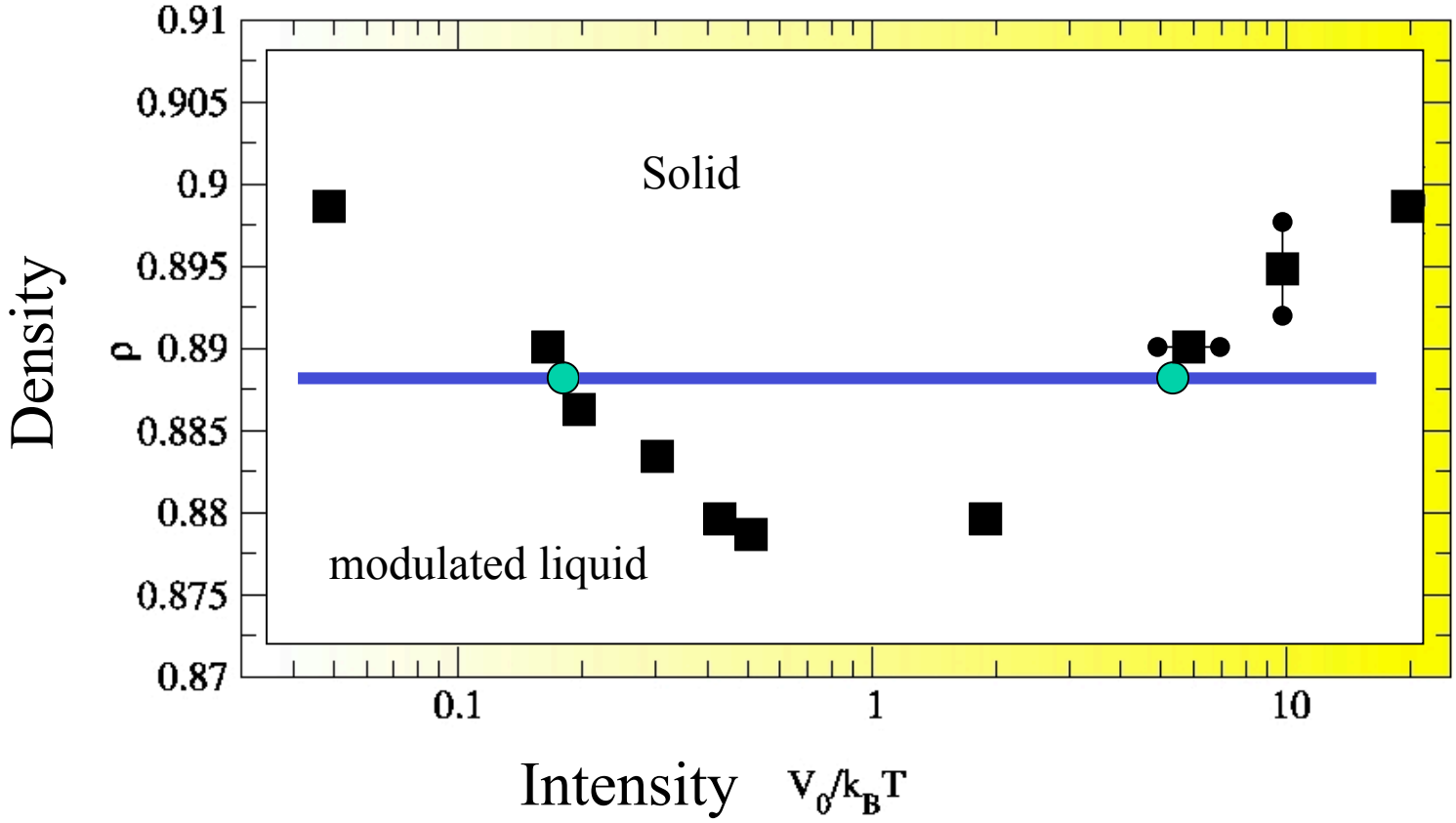

***Laser induced freezing***

# Suppression of fluctuations perpendicular to “valleys”: “decoupling” of particles in neighbor-“valleys” for large $V_0$

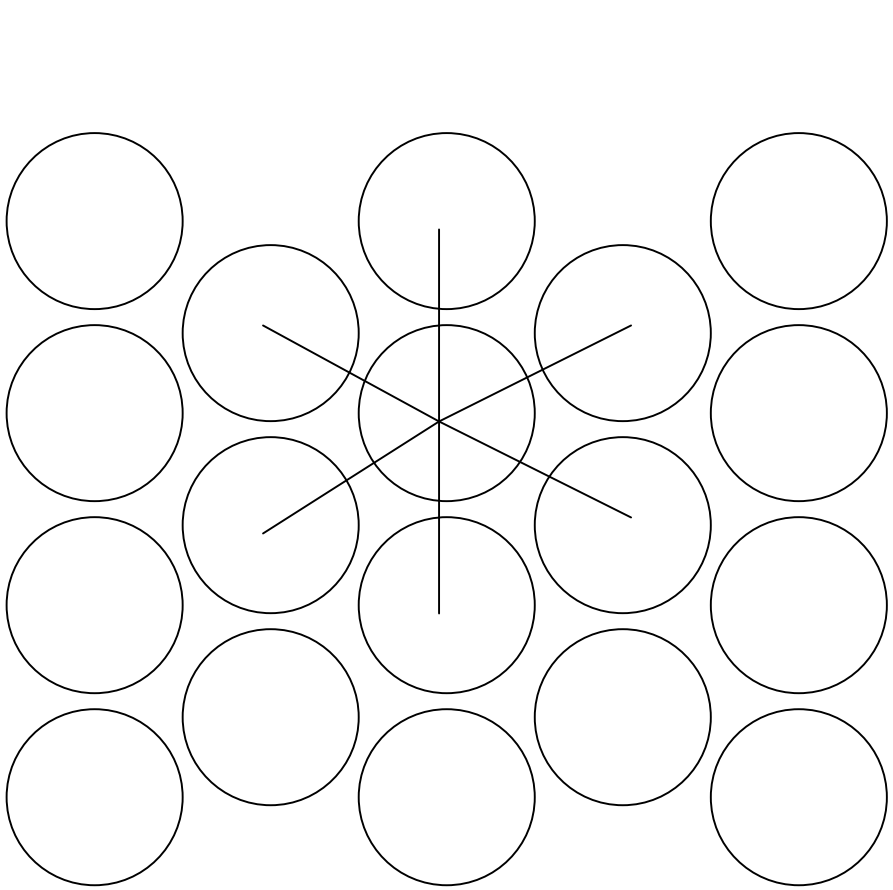



***Laser induced melting***

# Phase diagram (hard disks):



# Effect of the interaction range: interactions with “additional” neighbors



hard core interaction