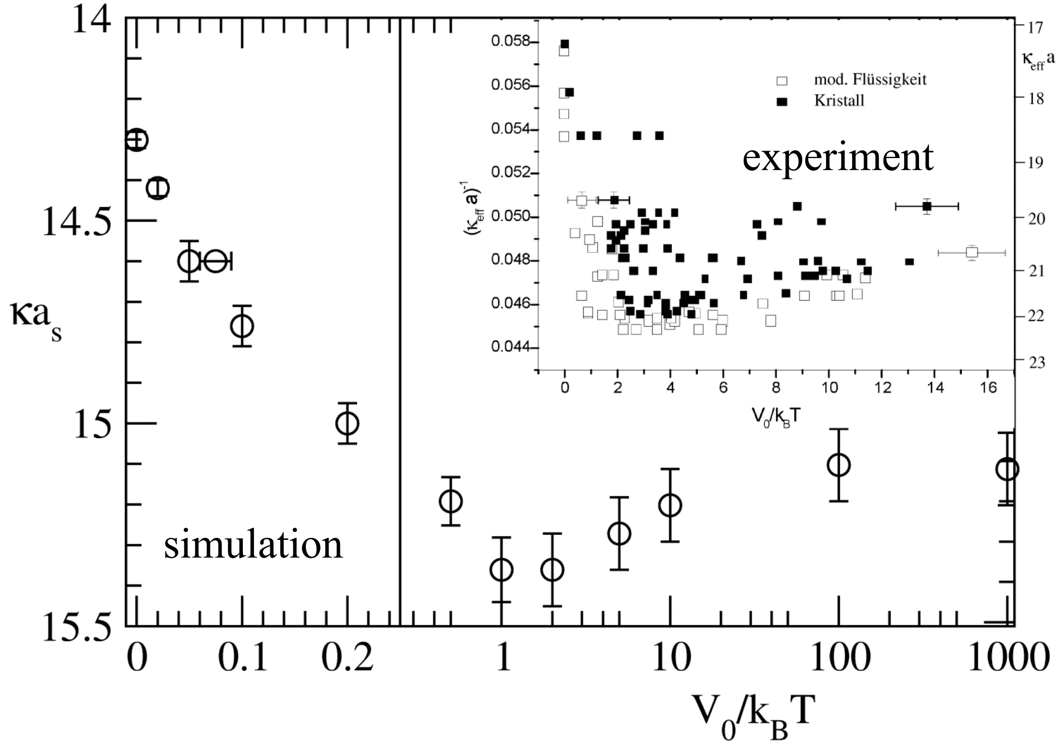
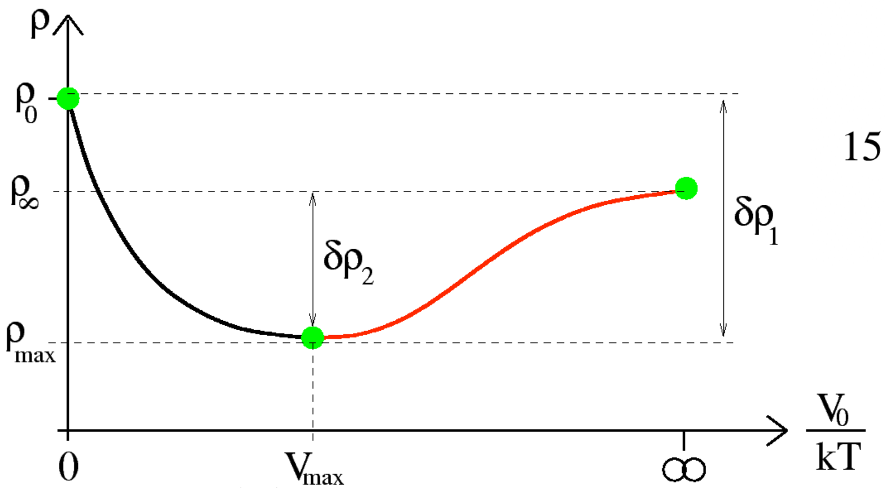
Phase diagrams: Effect of the potential range

DLVO-potential:
good qualitative agreement
with the experiment



Effect on reentrance:

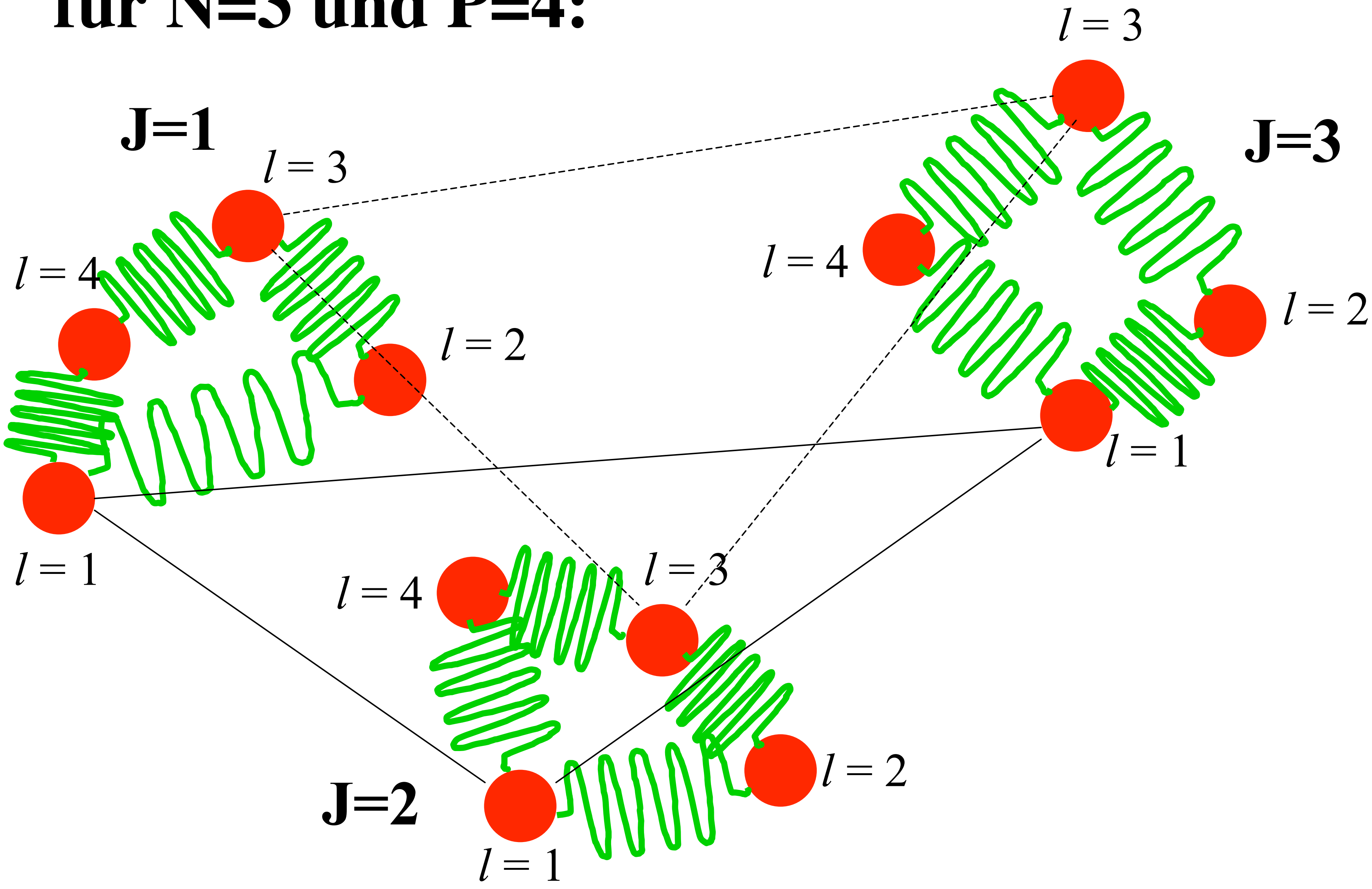


$$\Delta_{1,2} = \frac{\delta\rho_{1,2}}{\rho_0} = \frac{-2\delta(\kappa a_s)_{1,2}}{(\kappa a_s)_0}$$

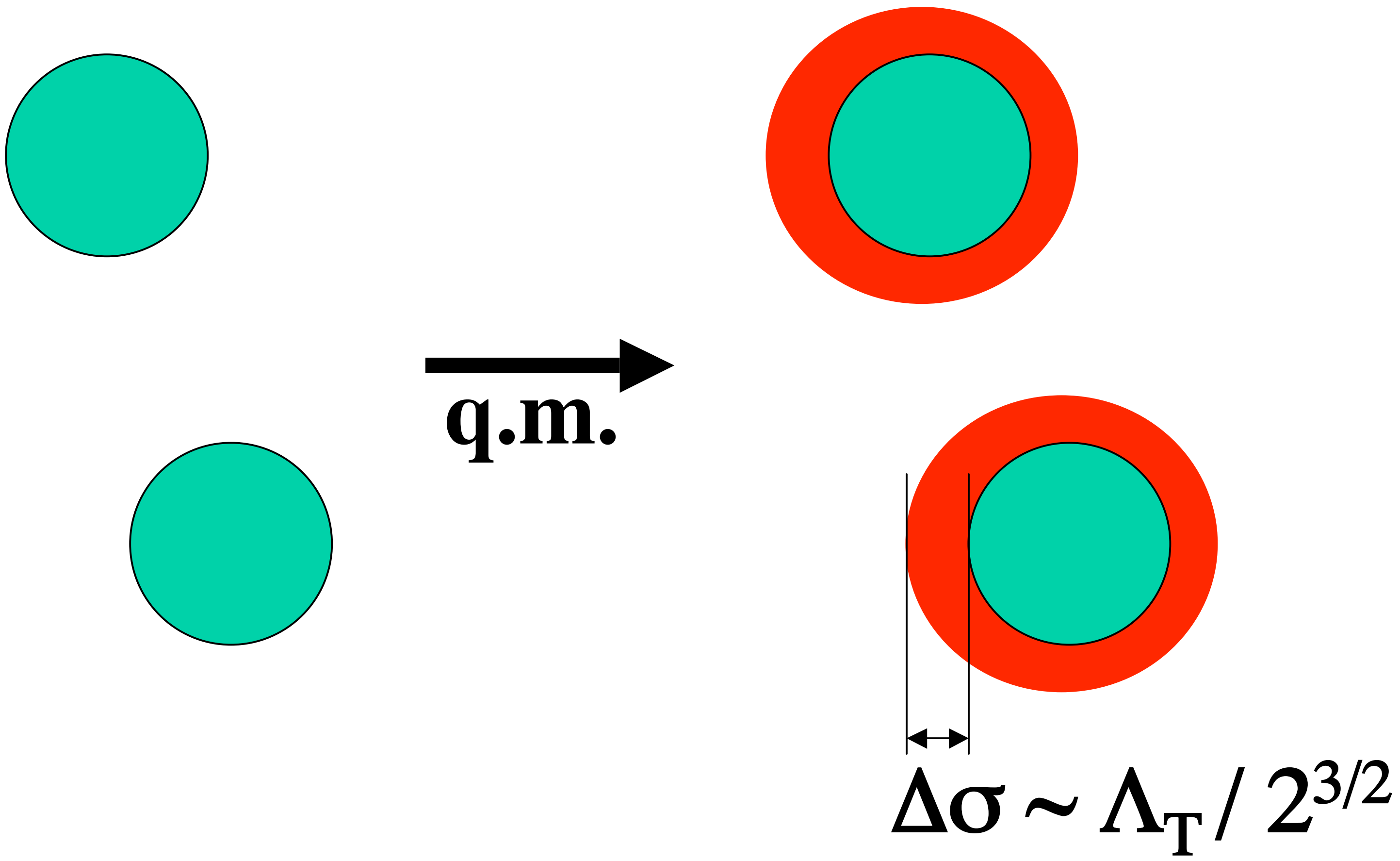
	Disks	DLVO	$1/r^{12}$	$1/r^6$	Expt. Colloids
Δ_1	0.043	0.149	0.091	0.182	0.55
Δ_2	0.028	0.034	0.027	0.007	0.185
Δ_1/Δ_2	1.53	4.63	3.37	26	3.91

Quanteneffekte für kleine Teilchenmassen?

Schema der „effektiven“ Wechselwirkungen für N=3 und P=4:

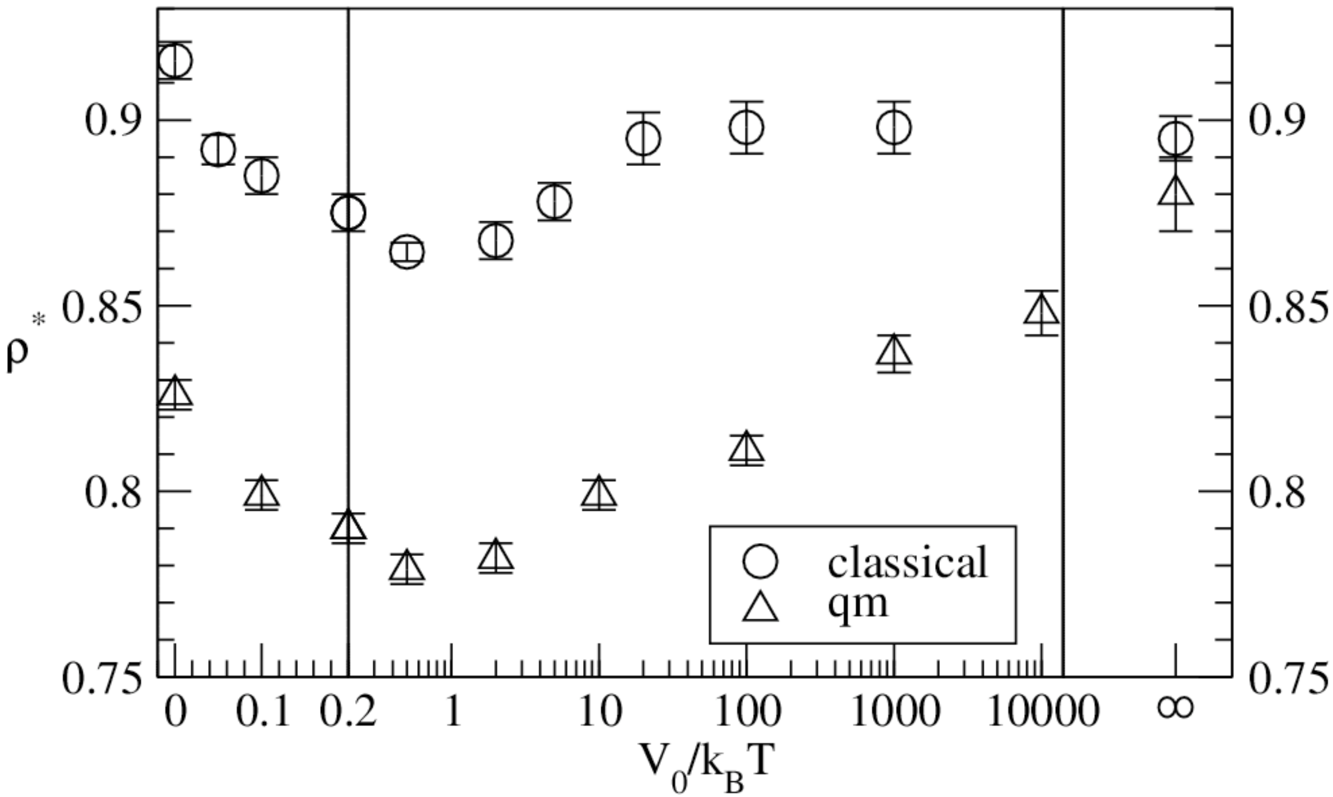


Zunahme des „effektiven“ harte Kugel-Durchmessers aufgrund der Orts-Impuls Unschärfe:



Quantum effects on the phase diagram :

Qualitative difference: quantum-melting (prediction!)



qm :

$PIMC\,(P = 64)$

$m^* = mT\sigma^2 = 10.000$

without ext. potential

with ext. potential

Colloidal dispersions:

Strukturen im Gleichgewicht:

Phasenumwandlungen und Quanteneffekte

Strukturbildung im Nichtgleichgewicht

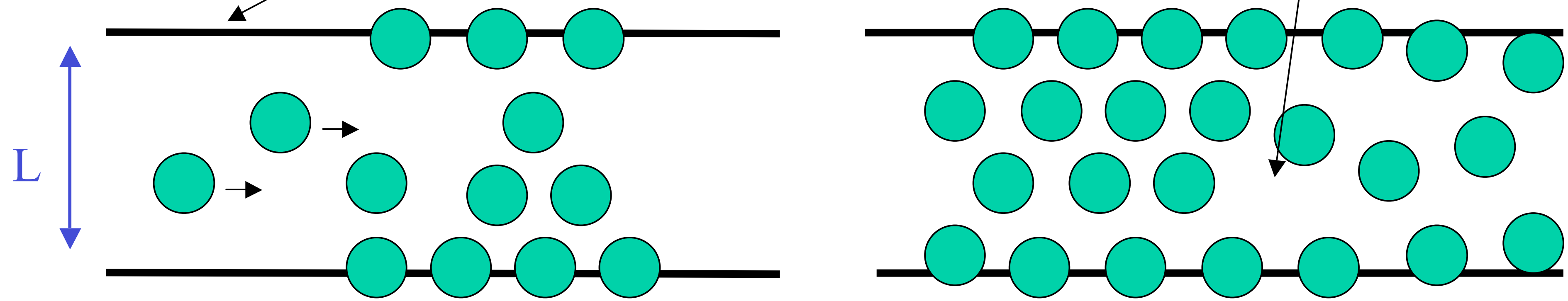
Vergleich mit Experimenten und Voraussagen

Structure formation in two dimensions

in confinement (walls)

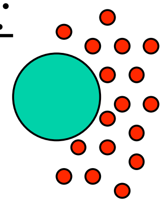
at defects

Layering and Lane Reduction:

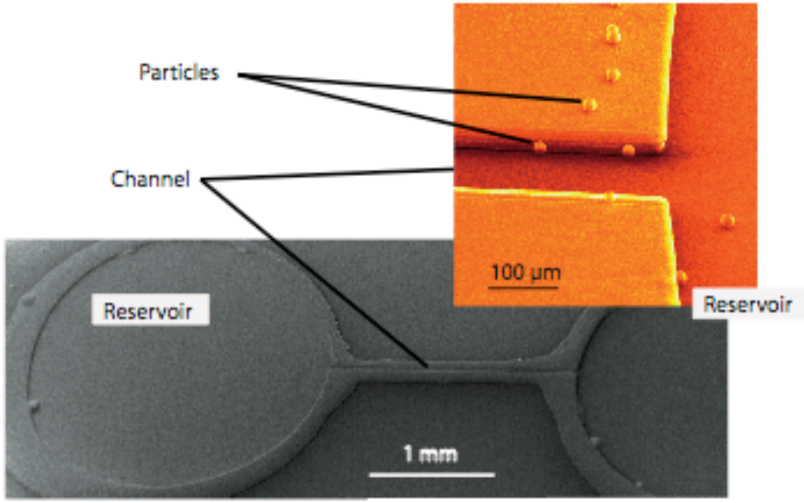


- Study and analysis of structure formation mechanisms
- Effects of geometry (L), diameter ratios, composition,
  density, temperature, flow velocity,…
- Comparison to three dimensional scenarios
- Test of thermodynamical approximations

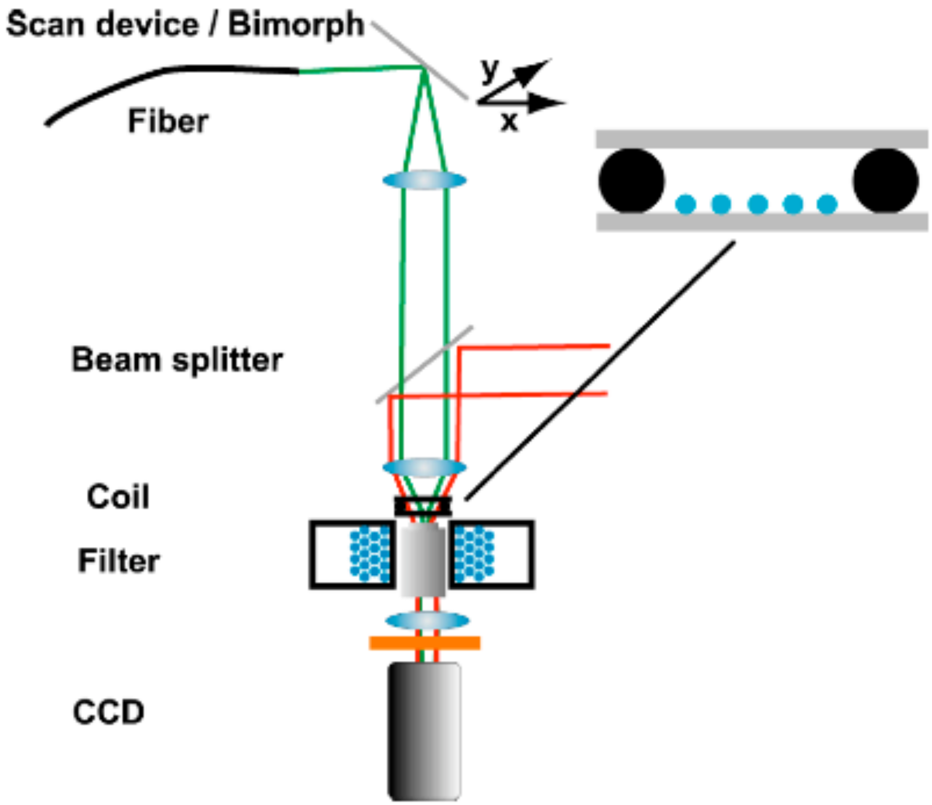
Mixtures:



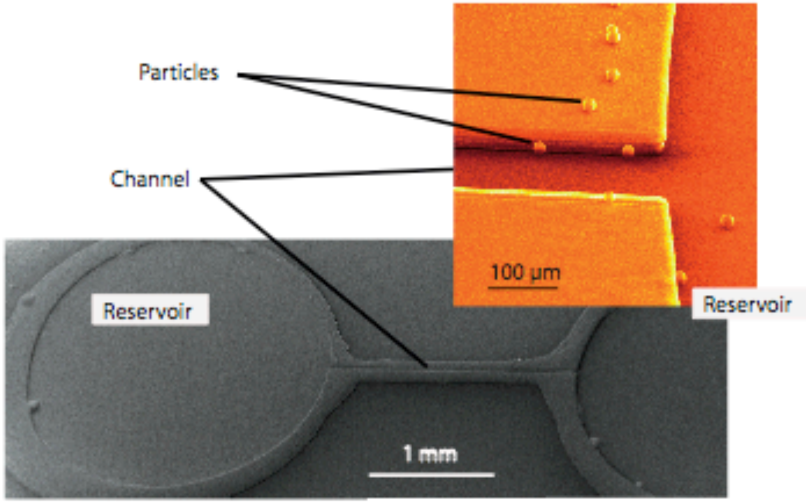
Video microscopy



- Colloidal suspension confined in a glass cell
- The particles settle to the lower surface of the glass cell (quasi 2d system)
- External potentials controlled by laser and magnetic fields.
- Confinement defined by optical lithography



Video microscopy



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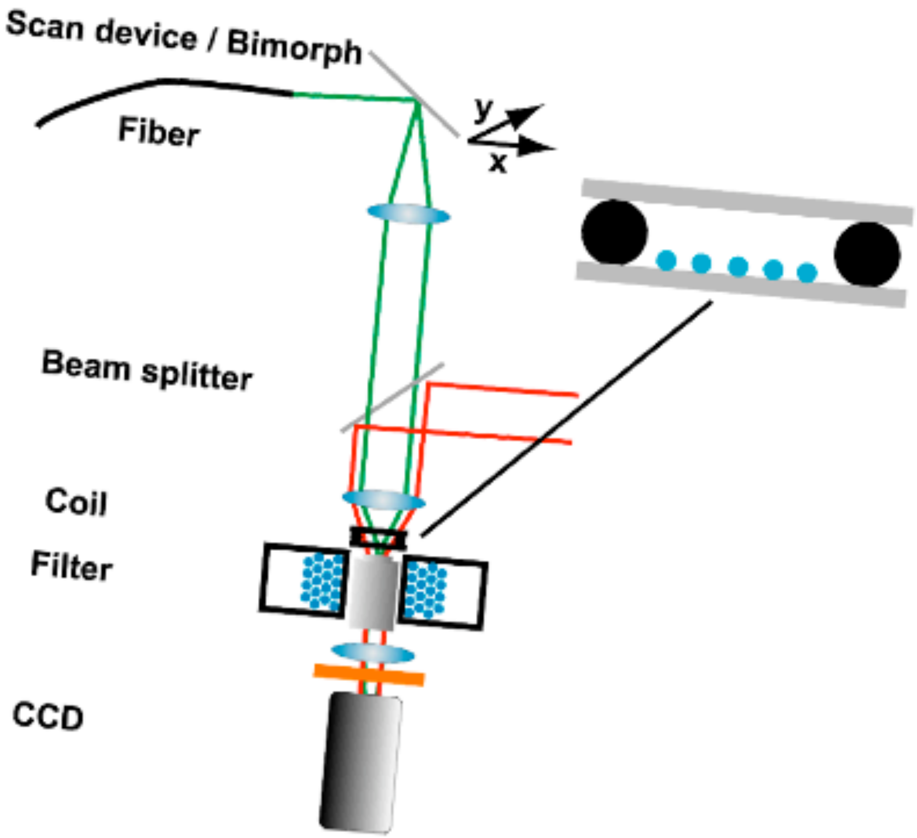


Layer formation of particles in a channel

tilt direction

Layer reduction →

8 layers

7 layers

$B = 0.24$ mT $\Rightarrow \Gamma \approx 72$

one image every 10 seconds

Method: Computer Simulations

N particles in finite volume at temperature T
(periodic boundary conditions / confinement)

- Molecular Dynamics
- Monte Carlo
- Brownian Dynamics

overdamped Langevin equation with drag coefficient $\xi = 3\pi\eta\sigma$

$$d\mathbf{r}_i(t) = \frac{1}{\xi}\left(-\nabla_{\mathbf{r}_i}\sum_{i\neq j} V_{ij}(r_{ij}) + \mathbf{F}_i^{\mathrm{ext}}\right)dt + \sqrt{\frac{2k_BT}{\xi}}\,d\mathbf{W}_i(t)$$

- stochastic differential equation, where $\mathbf{W}_i$ is a Wiener process with

$\langle d\mathbf{W}_i(t)\rangle = 0$ and $\langle dW_{i\alpha}(t)dW_{j\beta}(0)\rangle = \delta(t)\delta_{ij}\delta_{\alpha\beta}$

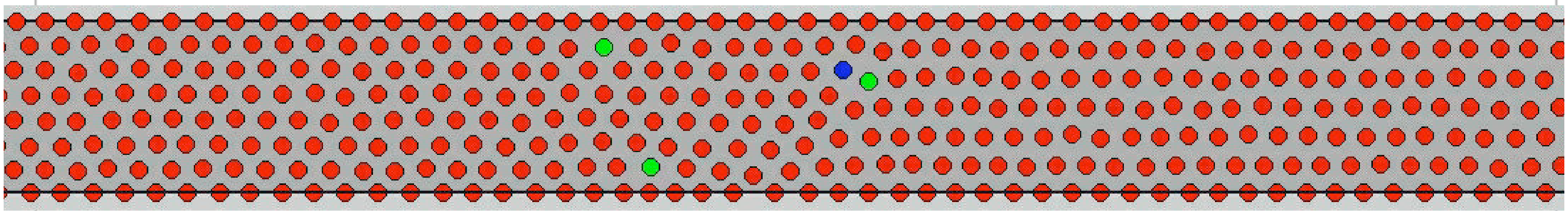
Pair interactions:

- Repulsive interactions (magnetic)

Brownian Dynamics simulation

- Starting configuration: random particle distribution
- Boundary conditions:
  - channel side walls and channel entrance are ideal hard walls
  - channel end is open
  - particle number N is kept fixed

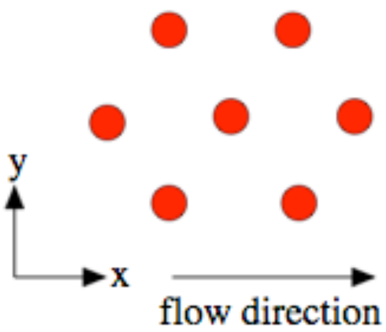
    ➡ insert a new particle at channel start, when a particle drops out

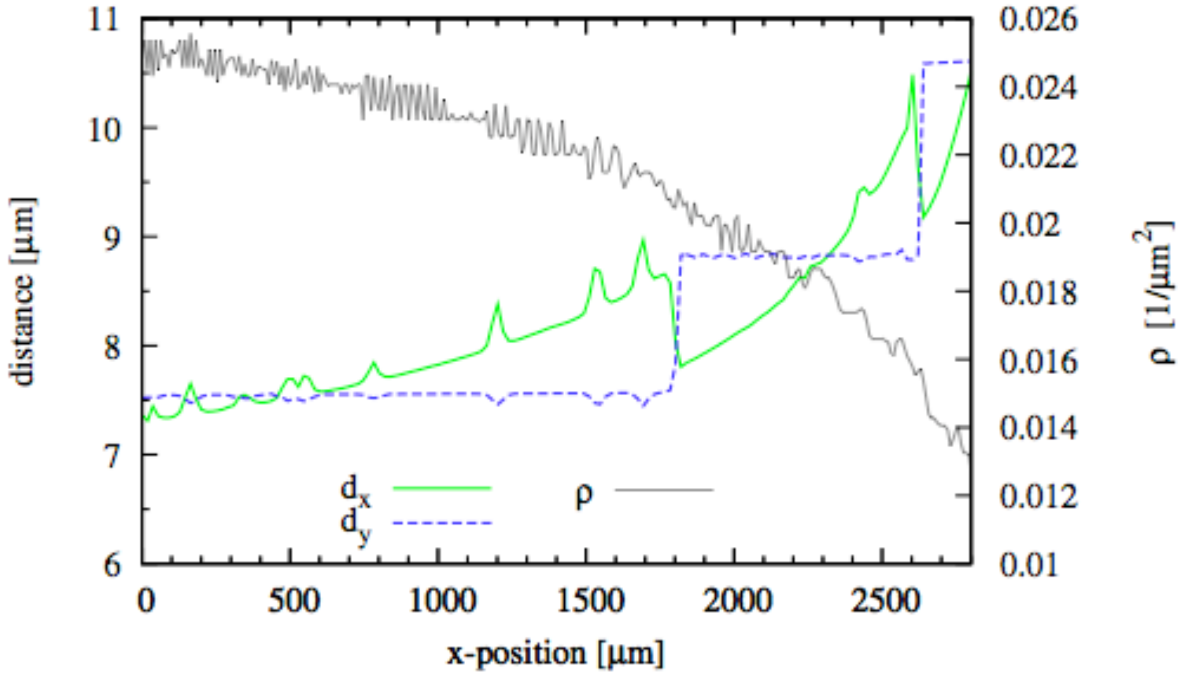


8 lanes $\rho = 0.4\sigma^{-2},\ \Gamma = 533.74,\ v_{\mathrm{drift}} = 0.035\ \mu\mathrm{m/s}$ 7 lanes

Layer reduction in the simulation

- Local lattice constants and local particle density in the **simulation**

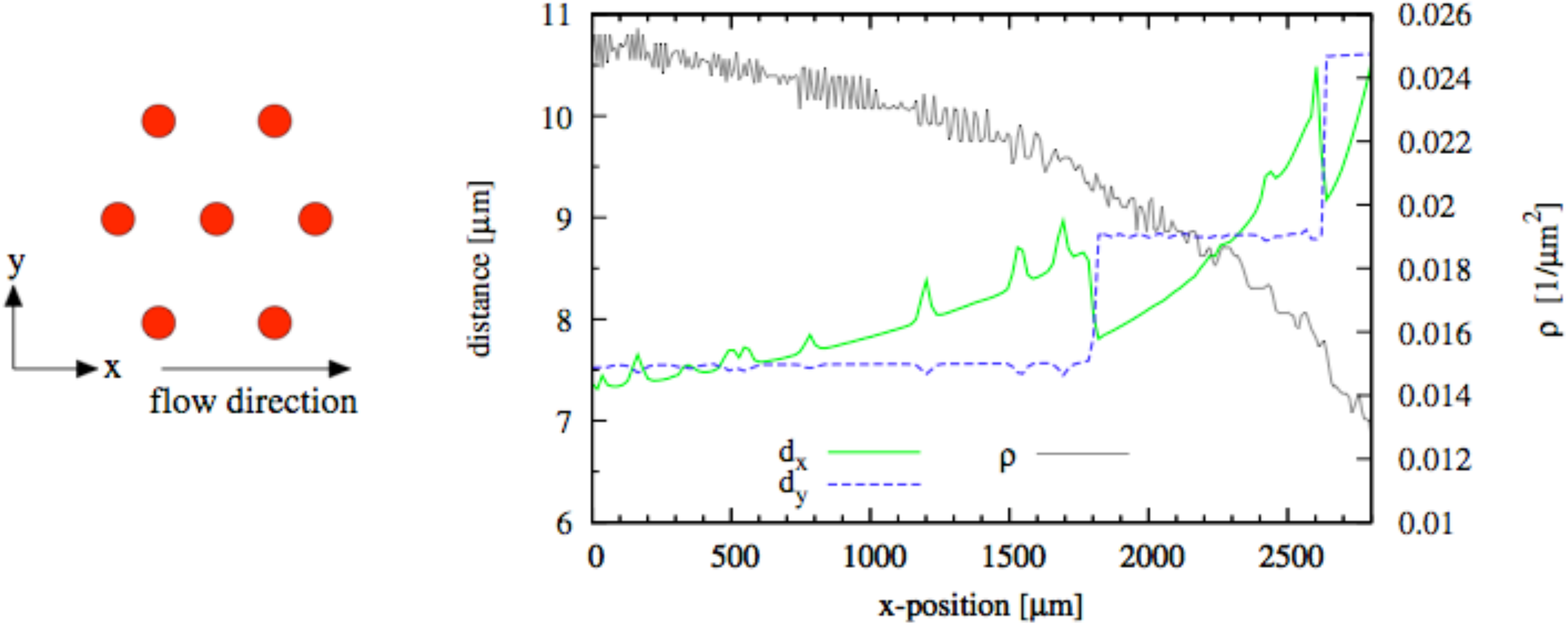




- continuous decrease of the local density
- stretched structure in flow direction before the point of layer-reduction and compressed structure afterwards

Layer reduction in the simulation

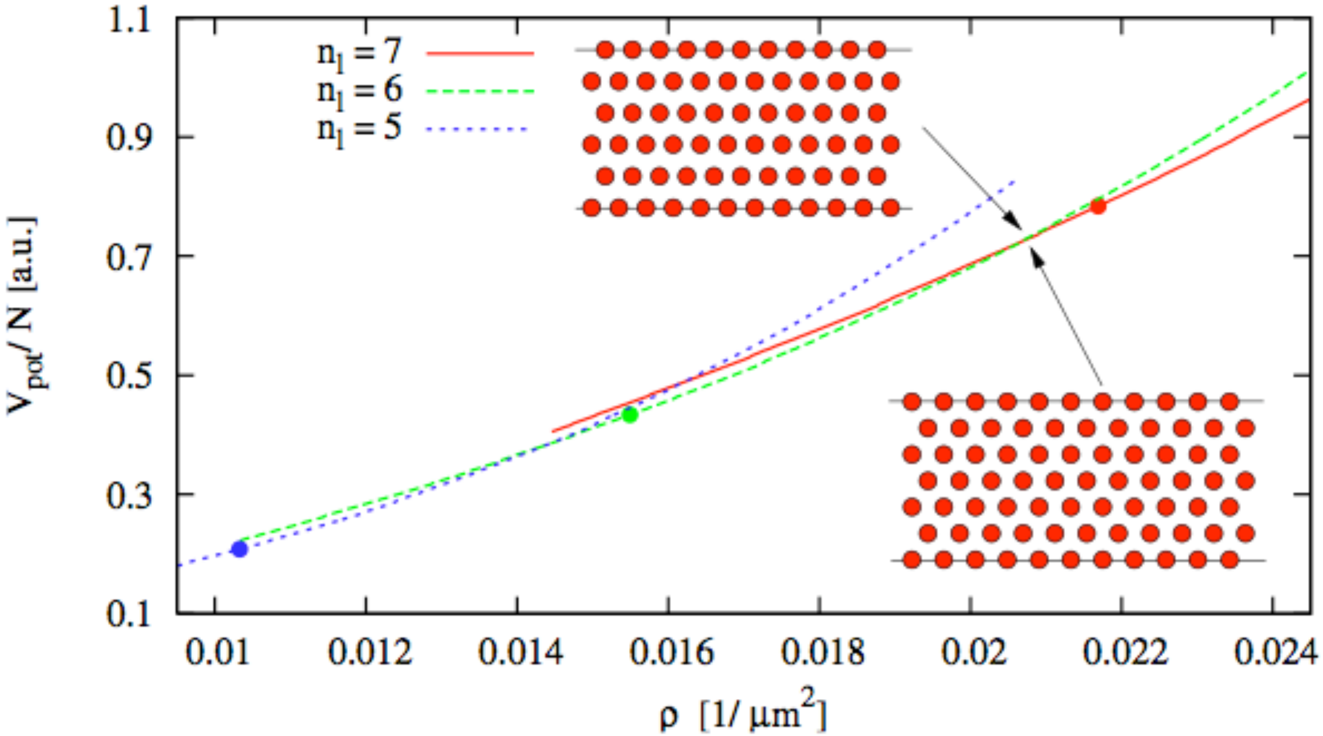
- Local lattice constants and local particle density in the **simulation**



- continuous decrease of the local density
- stretched structure in flow direction before the point of layer-reduction and compressed structure afterwards

Stretching the crystal - a rough estimation

- potential energy per particle obtained by scaling the channel length of different static configurations



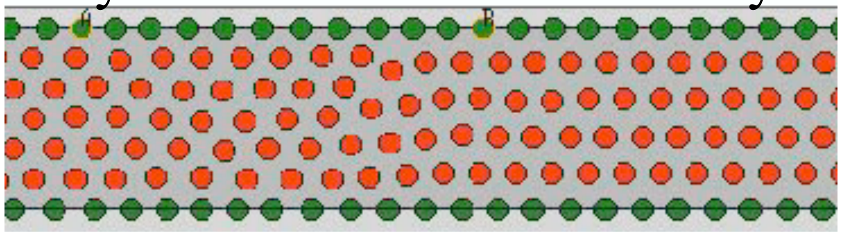
- Intersection points: crystal changes from one configuration to the more favorable

Recent cooperation with experimental projects (Erbe/Leiderer):

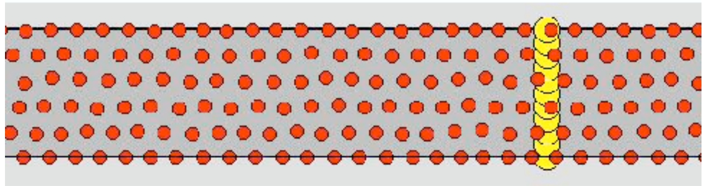
M. Köppl, P. Henseler, A. Erbe, P. Nielaba, P. Leiderer, Phys. Rev. Lett. **97**, 208302 (2006)

- *Layer reduction in 2D model colloids in gravitational fields:*

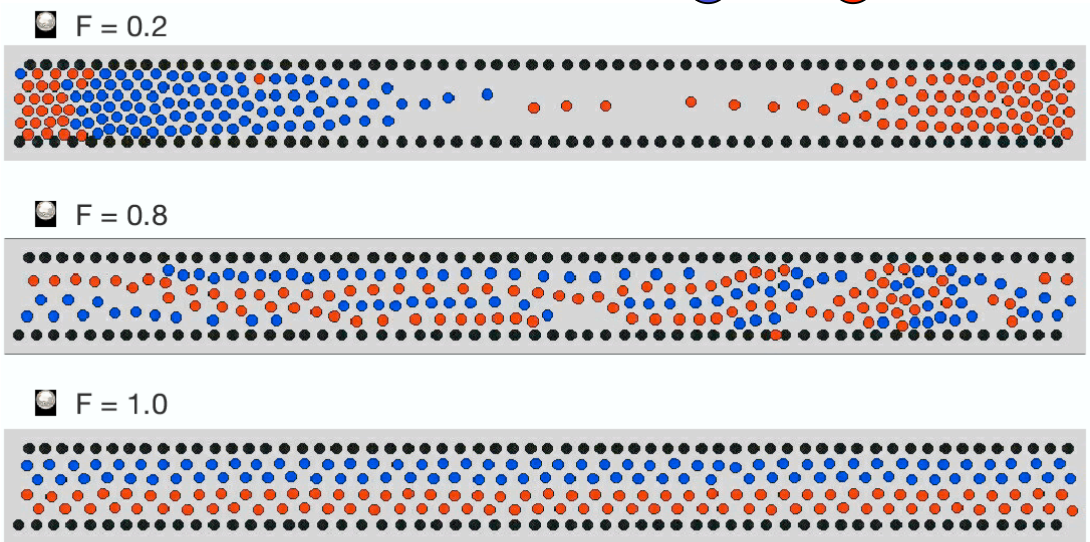
5 layers particle flow 4 layers

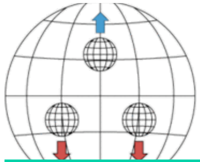
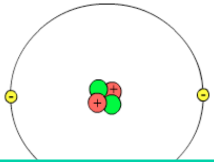
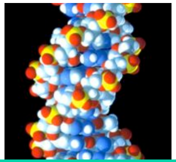


- *Structure formation at „walls" in flow direction:*



- *Effect of external driving forces (F) in binary model colloids:*



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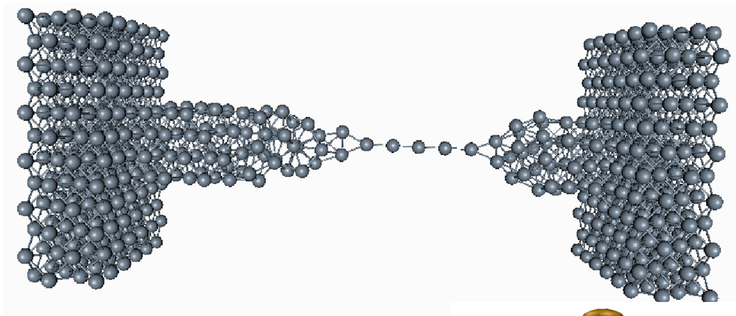
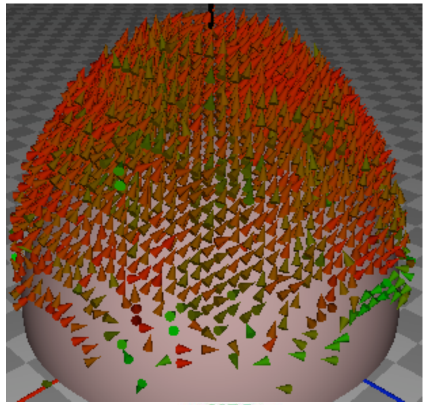
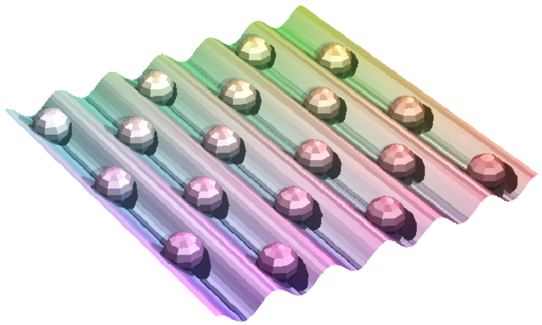
- Numerisch exakte Behandlung komplexer Systeme
- Überprüfung analytischer Näherungen
- Voraussagen fürs Experiment

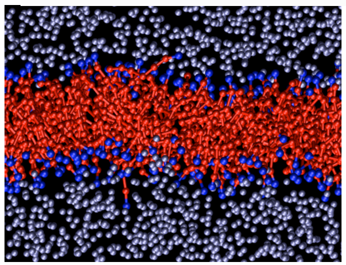
Vielteilchensysteme | **Quantenphänomene** | **Magnetismus**

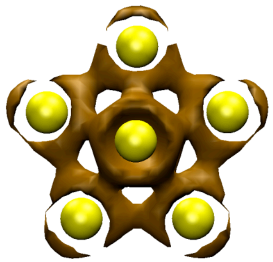
- Materialien für die Zukunft
- Nano-Bauelemente
- Neue Speichermedien
- Struktur-Änderungen durch äußere Felder

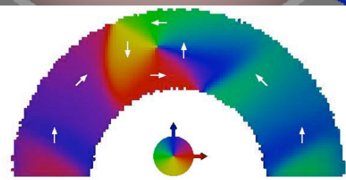




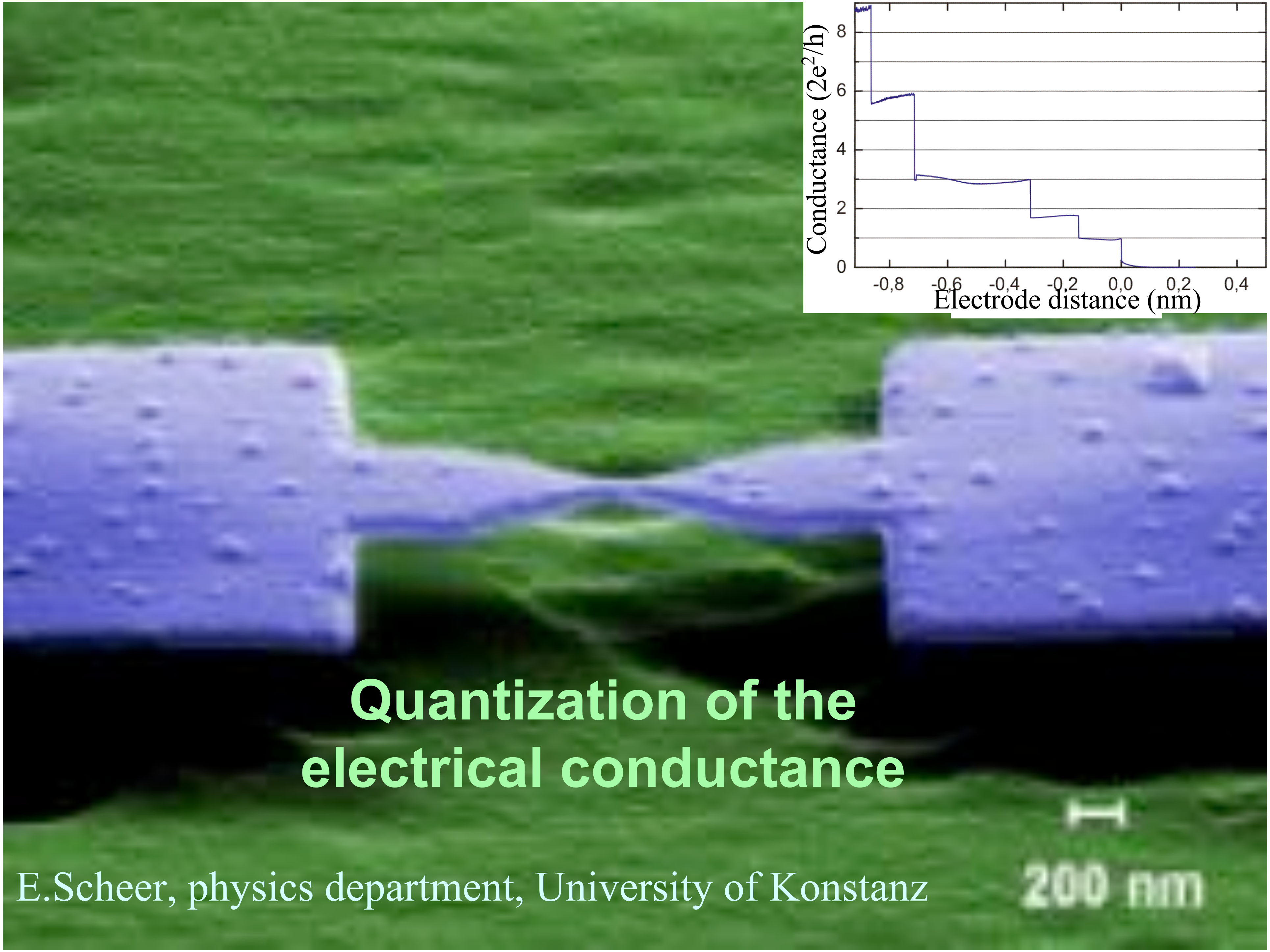








Nachbarwissenschaften: Mathematik (Modellbildung, Methoden), Informatik, Chemie (Moleküle), Biologie (Membran), Finanz-Physik (€)



Quantization of the electrical conductance

E.Scheer, physics department, University of Konstanz

Single-atom-contacts:

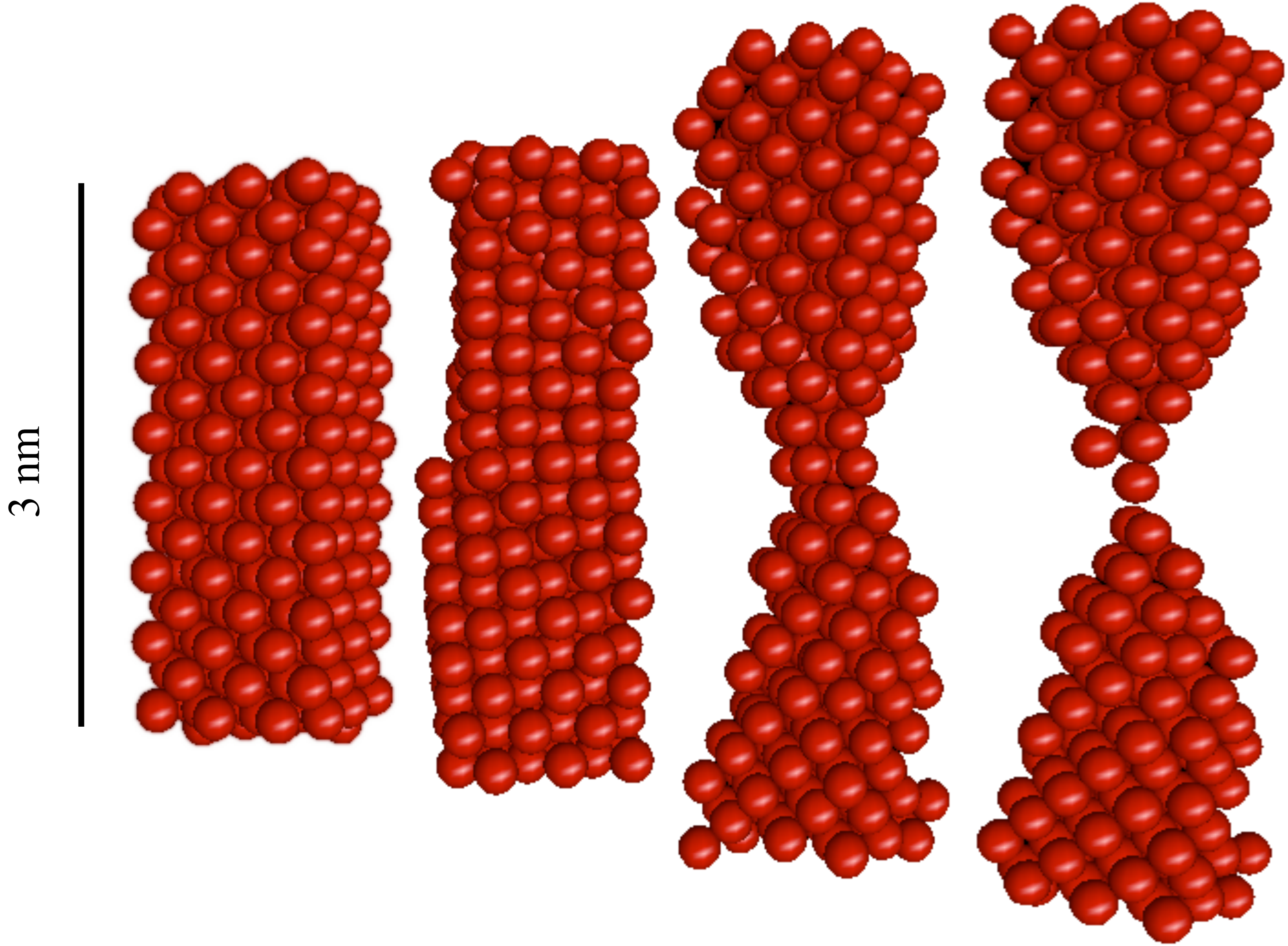
Electronic properties of Nano-materials can differ much from those of macroscopic systems (example: conductance-quantization (AG Scheer)

<u>Questions:</u>

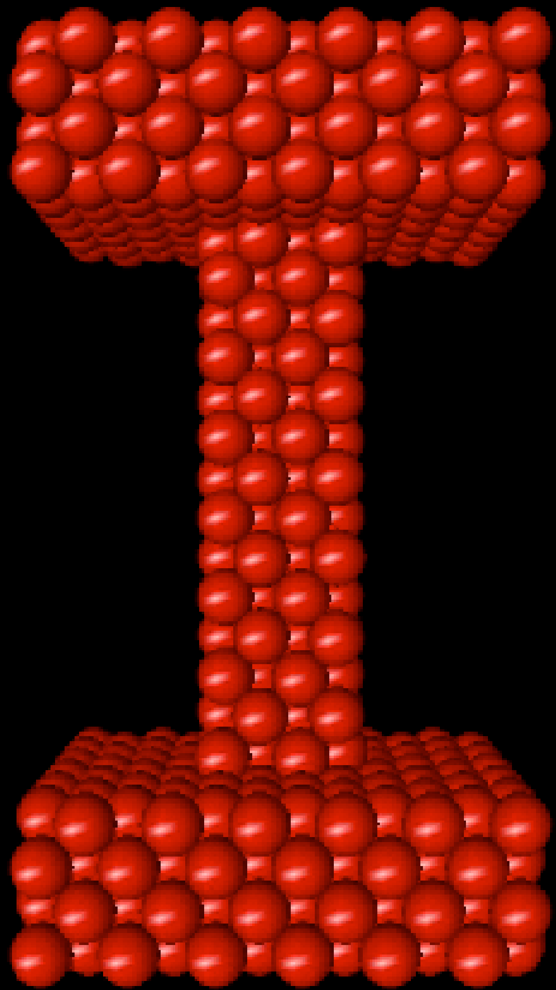
1) Formation process of single atom contacts ?
2) Current through these contacts ?

ad 1): MD-simulation of a stretching process in a Au-wire (M. Dreher)
(Au-wire, 300 atoms, oriented in (100) direction)

ad 2): Computation of current in these configurations
Method: tight binding, thermal average
(cooperation with C. Cuevas, J. Heurich and E. Scheer)


3 nm

Simulation
of a stretched
gold wire



Conductance-quantization in single-atom contacts:

- Conductance-quantization in transport-„channels“ due to the wave-nature of the electrons (see „box-potential“):

$$G = I/V = \left[ev(\partial n/\partial E)(\mu_1 - \mu_2)T\right]/\left[(\mu_1 - \mu_2)/e\right] = \left(2e^2/h\right)T \qquad \text{(one channel)}$$

$$G = \left(2e^2/h\right)\sum_{i=1}^{N} T_i \qquad \text{(N channels)}$$

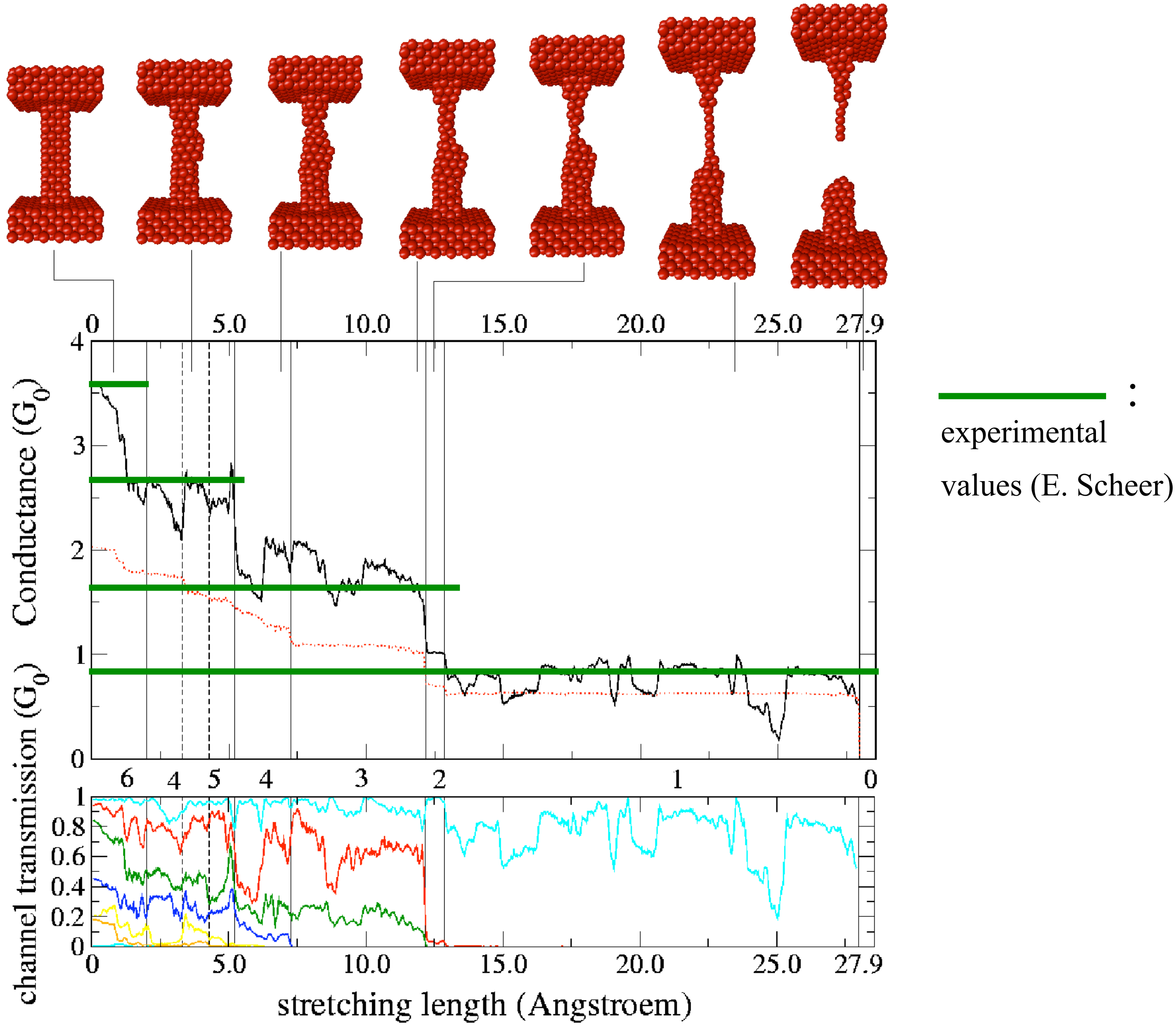
$$G_0 = \left(2e^2/h\right) \qquad \text{(Landauer-Büttiker-formalism, PRB31,6207 (85))}$$

- Computation of G in „tight-binding“ - approximation:

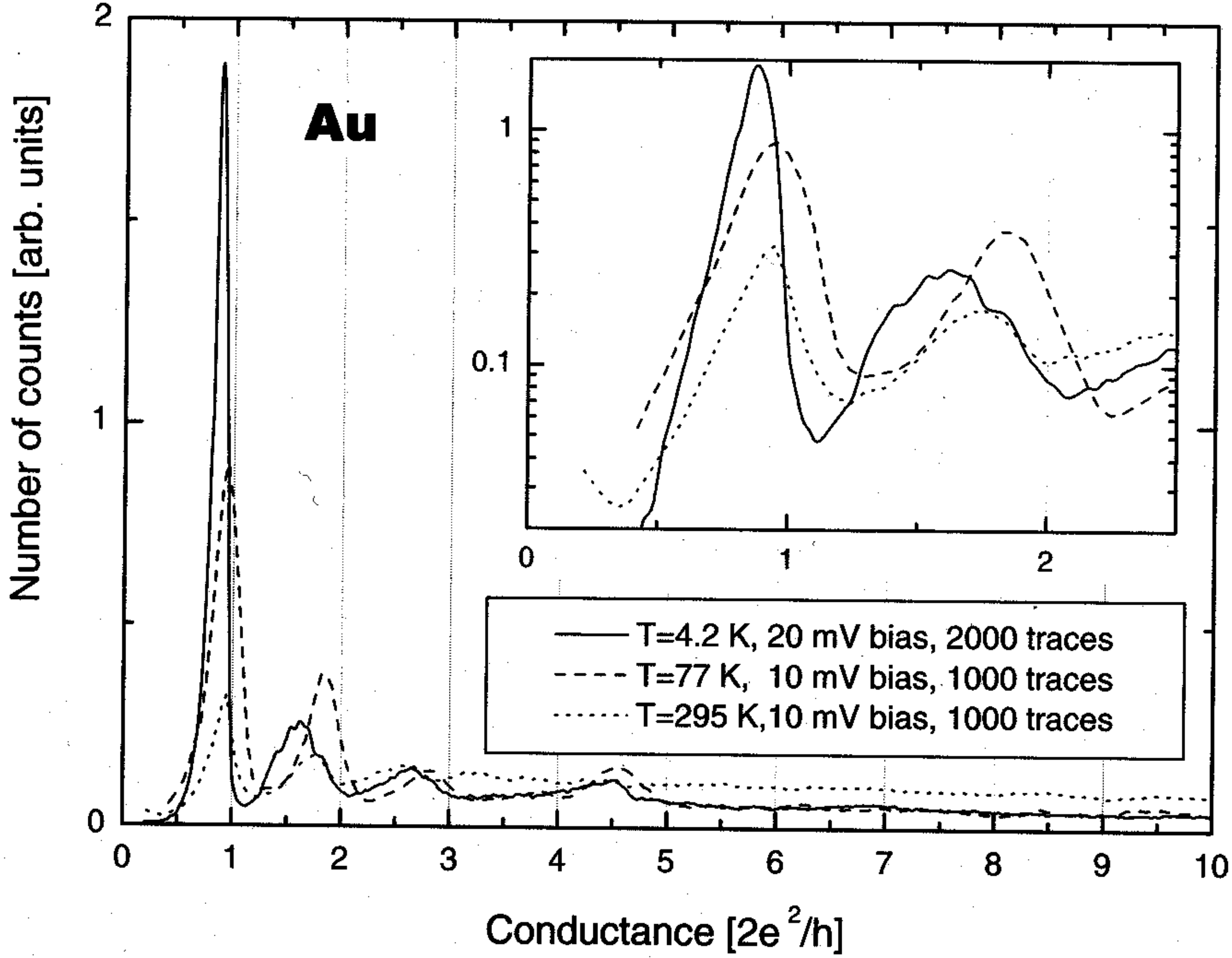
$$H = \sum_{i\alpha,\sigma} \varepsilon_{i\alpha} c^{+}_{i\alpha,\sigma} c_{i\alpha,\sigma} + \sum_{i\alpha \neq j\beta,\sigma} t_{i\alpha,j\beta} c^{+}_{i\alpha,\sigma} c_{j\beta,\sigma}$$

$$G = (2e/h)\,Tr\left(\hat{t}\hat{t}^{+}\right) \quad , \quad \hat{t}\hat{t}^{+} - Matrix\ with\ N\ Eigen\ values\ T_i \quad , \quad G = G_0 \sum_{i=1}^{N} T_i$$

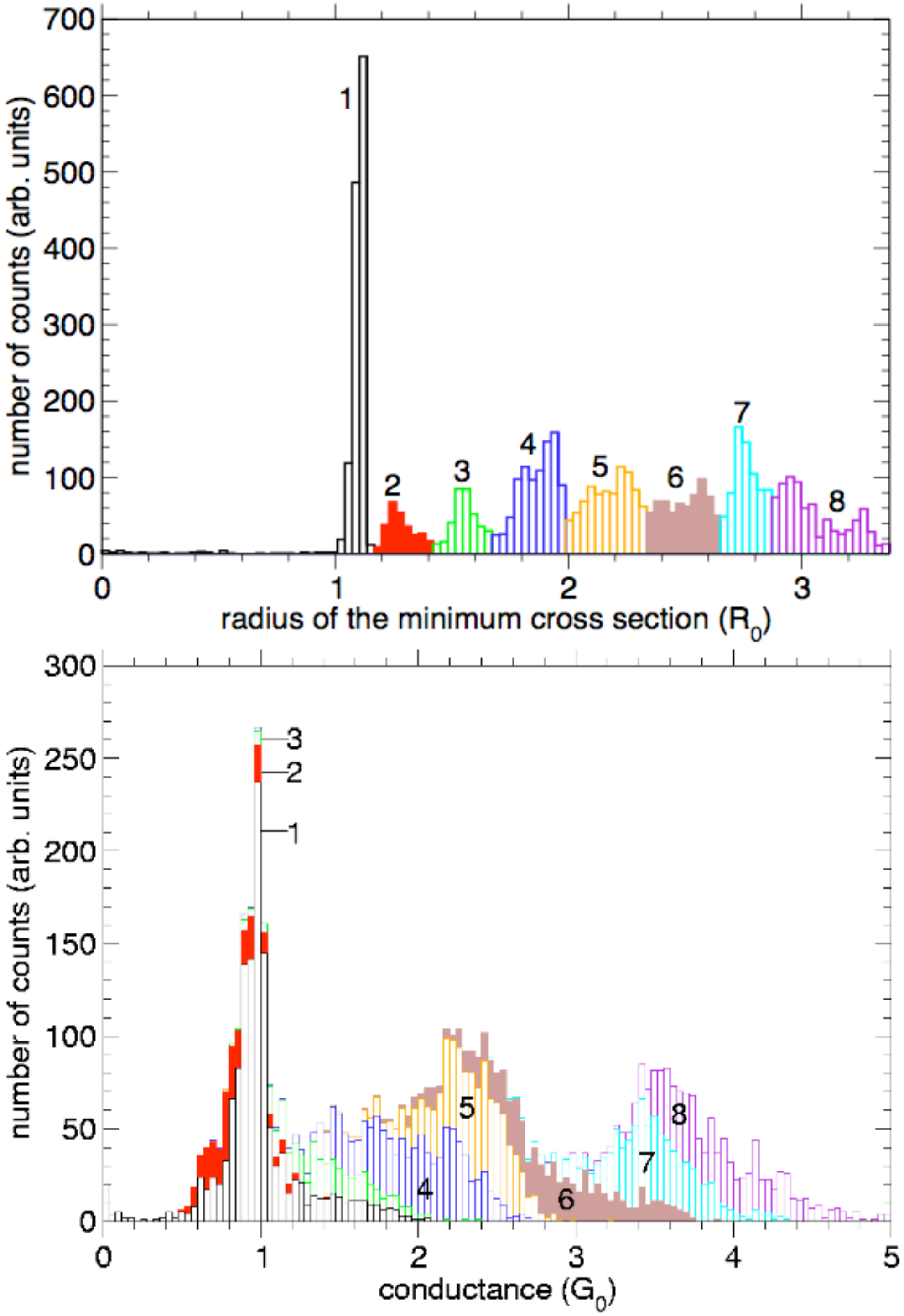
(Levy Yeyati et al., PRB56, 10369 (97), Cuevas et al., PRL80, 1066 (98))



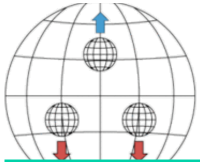
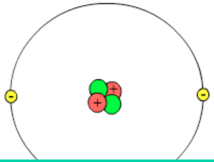
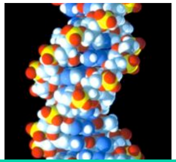
experimental
values (E. Scheer)
Conductance (G0)
channel transmission (G0)
stretching length (Angstroem)
0
5.0
10.0
15.0
20.0
25.0
27.9
6
4
5
4
3
2
1
0



Aus: A.I. Yanson, „Atomic chains and electronic shells: quantum mechanisms for the formation of nanowires“ Ph.D. thesis, Leiden (2001).



number of counts (arb. units)
radius of the minimum cross section (R0)
1
2
3
4
5
6
7
8
number of counts (arb. units)
conductance (G0)

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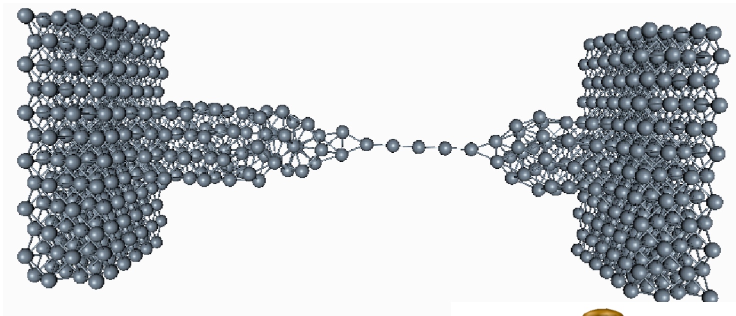

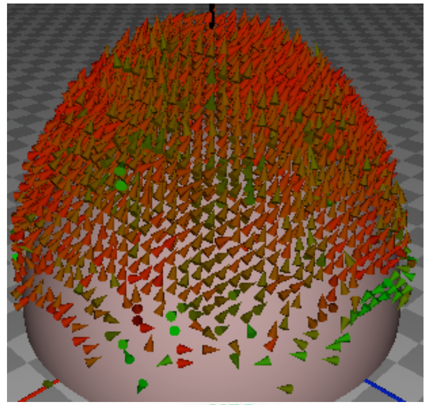

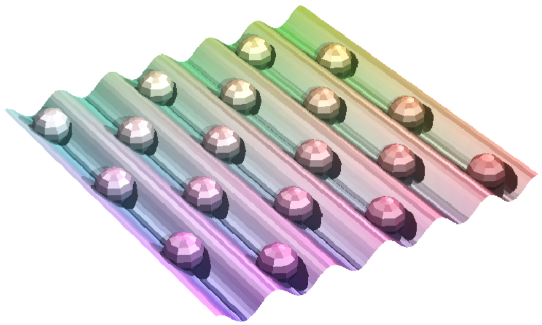

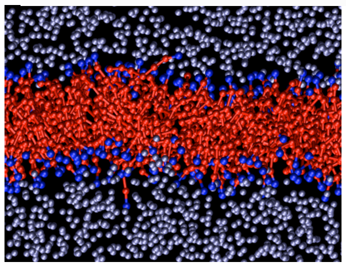

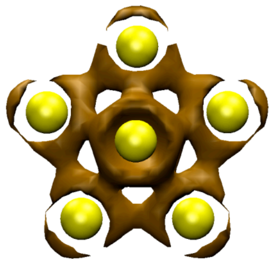

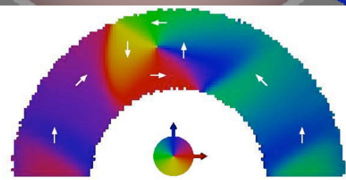

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