Ising Droplets in Action

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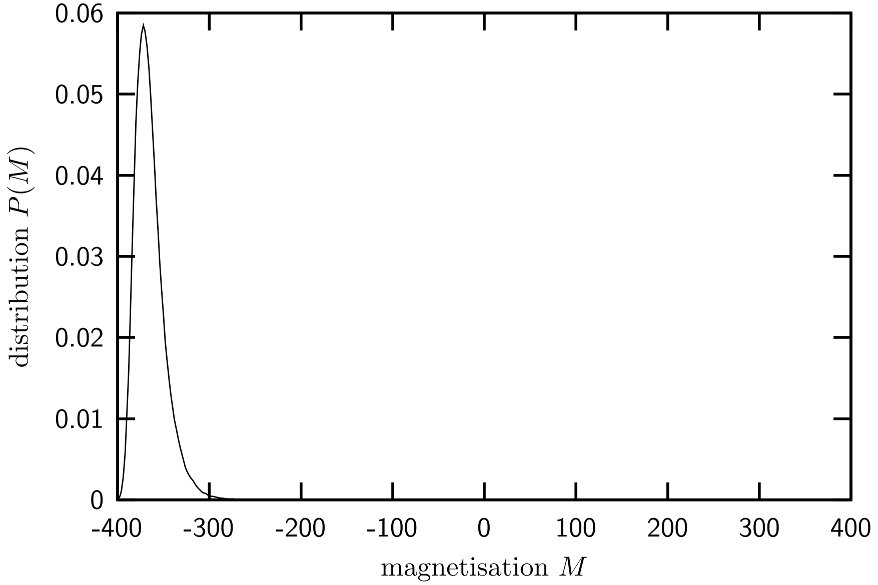
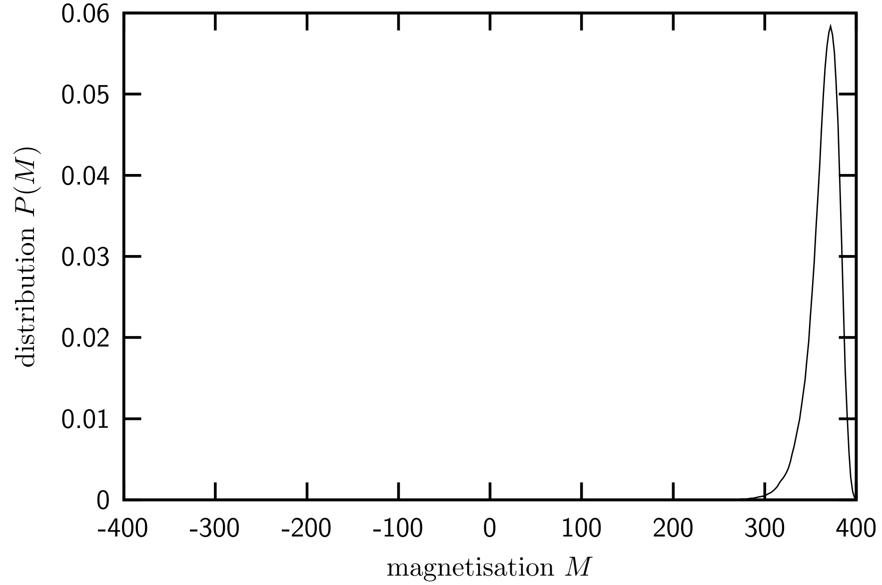
1 Motivation

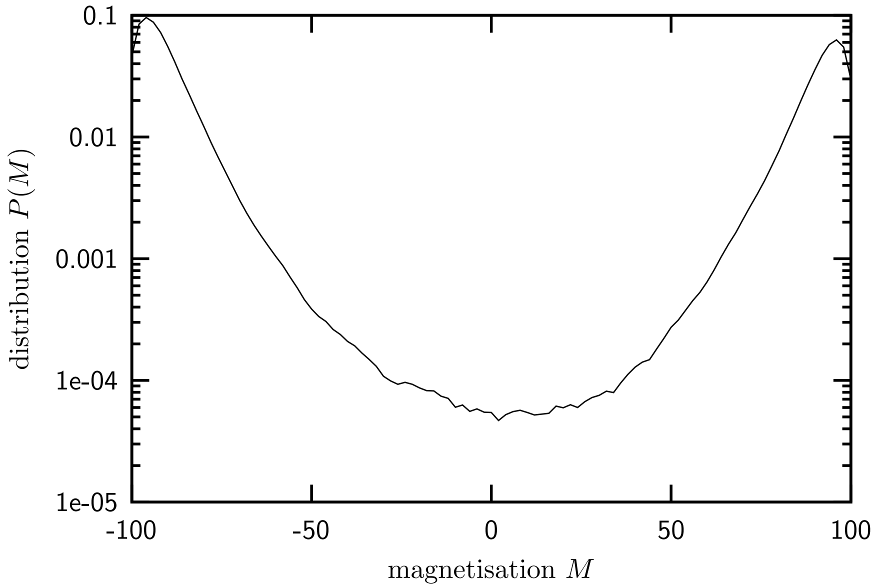
- Magnetisation of 2D-Ising simulation below $T_c = 2/\log(1+\sqrt{2}) \approx 2.269...$

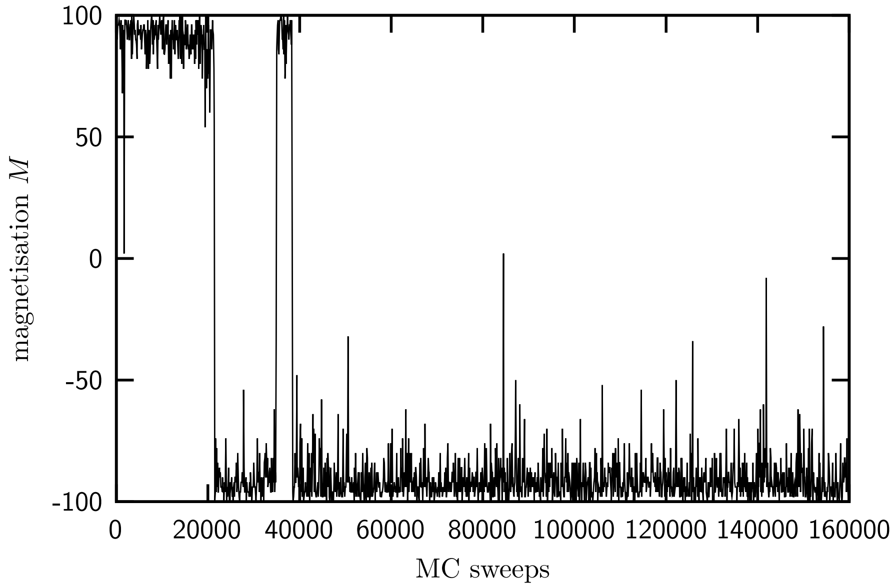




- When system size L is large enough (here: $L = 20$) and the temperature low enough (here: $T = 2.0$) simulation is trapped in states with positive/negative net magnetisation.
- The peak is located at $\pm M_{\rm sp}$ as predicted by Onsager/Young.
- The valley scales like $\exp(-\beta\sigma L) \Rightarrow$ transition time scales like $\exp(+\beta\sigma L)$.

- To see a transition between the peaks a fairly small system is simulated ($L = 10$, $T = 2.0$):



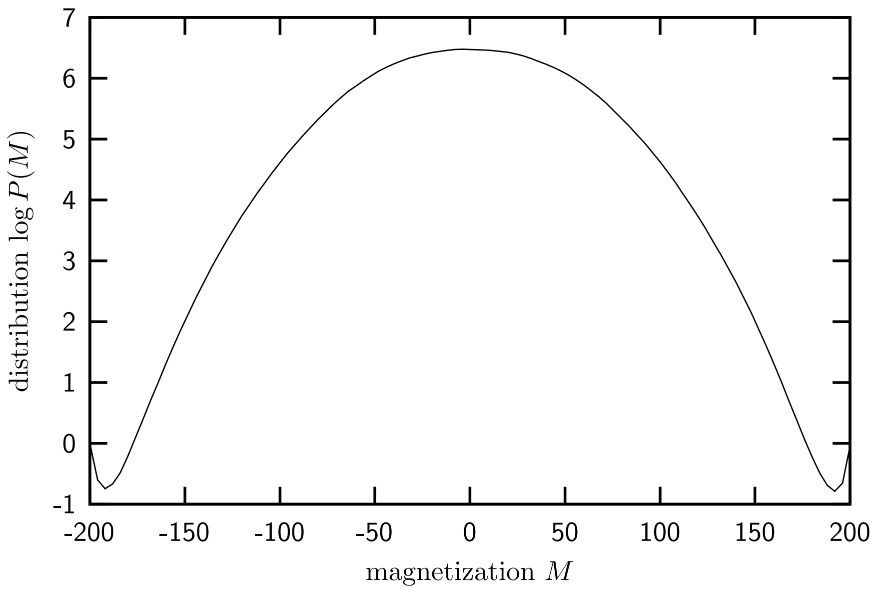


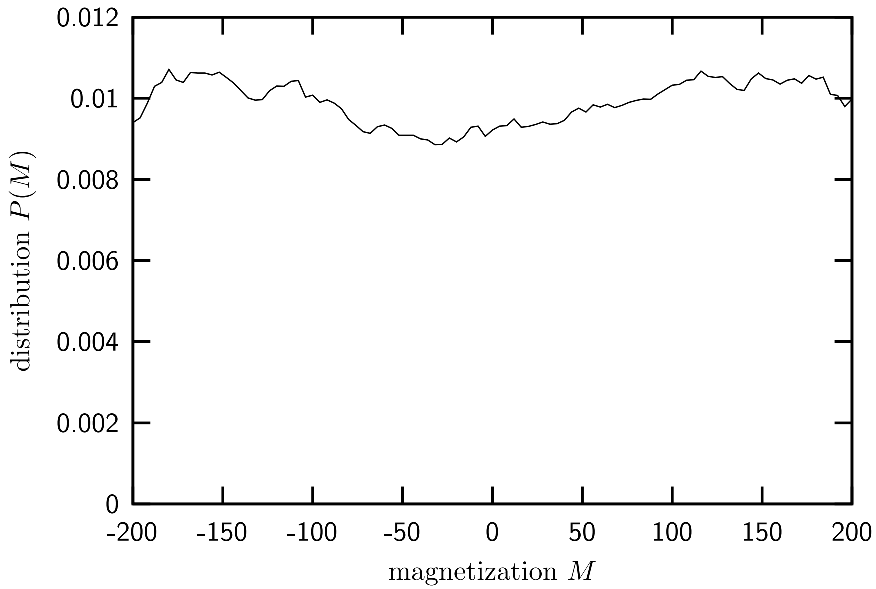
- From histogram: both peaks are visited and the valley is approximately suppressed by a factor $10^{-4}/10^{-1} = 10^{-3}$.
- From the time series: the transitions $-M_{\mathrm{sp}} \leftrightarrow M_{\mathrm{sp}}$ are visible as distinct jumps.
- Question: scaling of the valley, ... $\Rightarrow$ value $P($ M=0 $)$ is needed.
- Solution: Multicanonical algorithm (Berg and Neuhaus 1992)

2 Detour: the Mu(lti) Ca(nonical) algorithm

- Metropolis ≡ importance sampling: samples are drawn from the peaks of the distribution according to the Boltzmann distribution.
- Muca: sample are drawn according to a arbitrary auxiliary distribution.
- Relation between canonical and muca distribution:

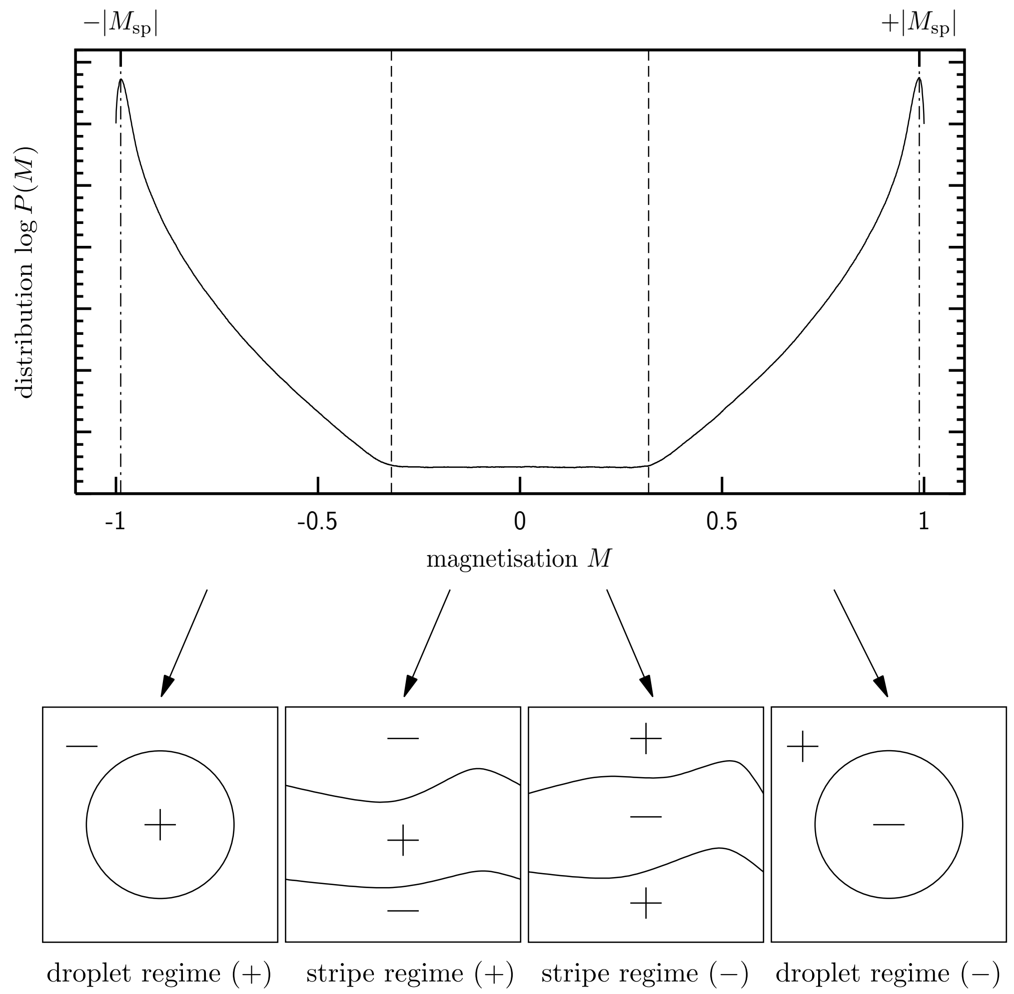
$$P_{\text{muca}}(M) \equiv P_{\text{can}}(M)\exp(-\beta f)$$



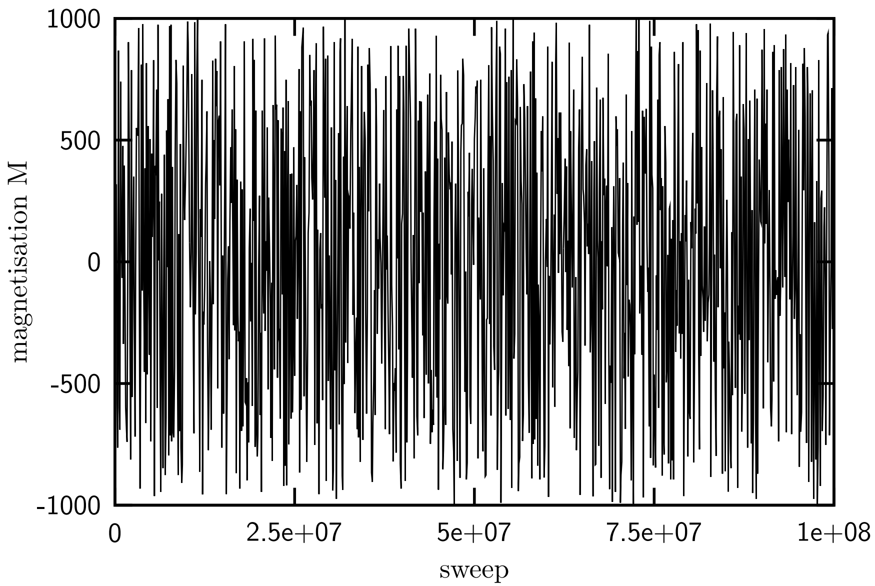


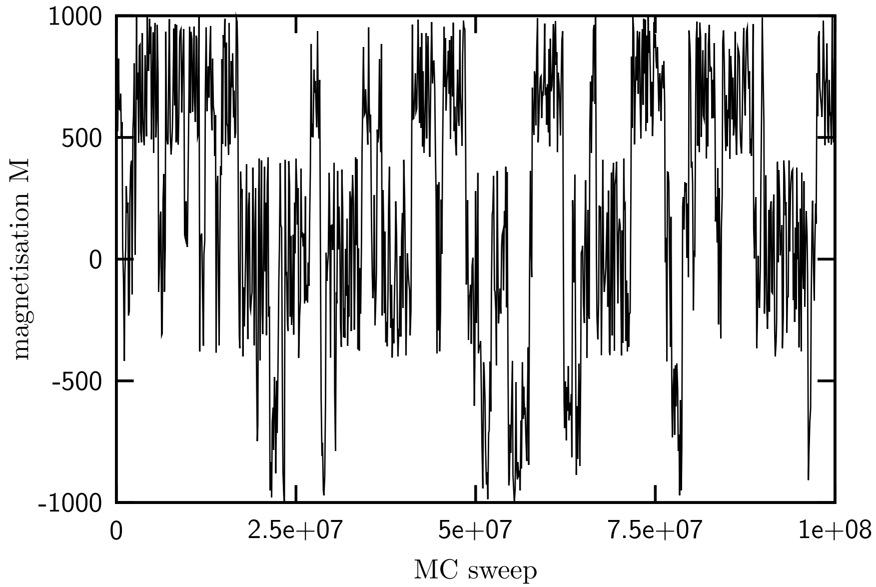
3 Return to motivation

- Well known plot of the distribution of the magnetisation, obtained with the MuM routine:



- Time series of MuM (Muca $\Rightarrow$ energy E, MuM $\Rightarrow$ magnetisation M) for a $10 \times 10 \times 10$ system (3D: $T_c \approx 4.51\ldots$) at $T = 2.5$ and $T = 2.0$:





- Left plot: erratic movement in the magnetisation ✓
  Right plot: blocked structure ✗

- Conclusion: there are hidden barriers (in the free energy) that cannot be removed (even with perfect MuM-weights[a]). ($\Leftarrow$ Stage of affairs up to 2002.)

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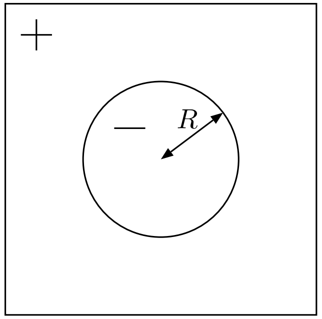
[a] Enumeration, extensive MuM-recursion, ...

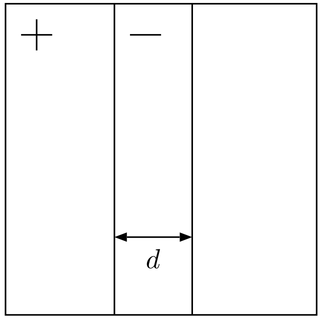
- In 2002: Neuhaus and Hager (cond-mat/0201324) explain this behaviour by a geometric first-order phase-transition.

- To understand this ⇒ Leung and Zia (1990): (m_0: spontaneous magnetisation, f_0: bulk free energy; simplification: $\sigma_\mathrm{S} \equiv \sigma_\mathrm{D} \equiv \sigma$, i.e. droplet and stripe have the same isotropic interface tension)

Droplet:



Stripe:

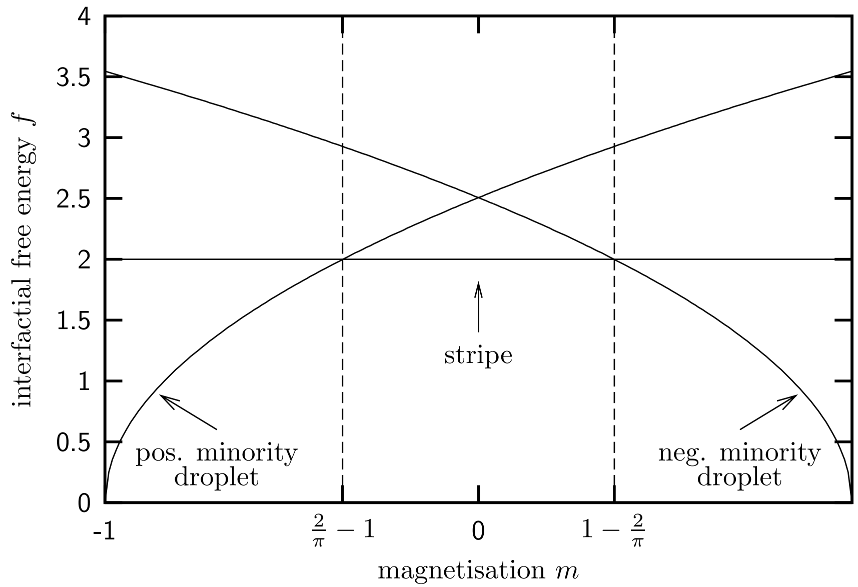


$$M_\mathrm{D} = m_0(L^2 - 2\pi R^2) \qquad M_\mathrm{S} = m_0(L(L-d) - dL) = m_0(L^2 - 2dL)$$

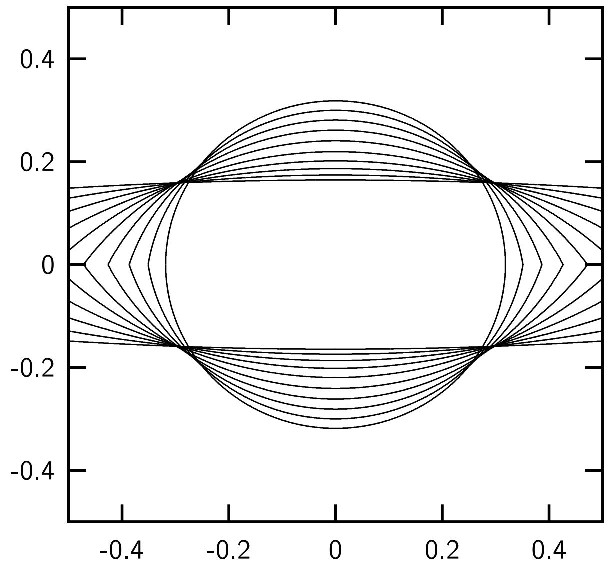
$$f_\mathrm{D} = f_0 + 2\pi R\sigma \qquad f_\mathrm{S} = f_0 + 2L\sigma$$

Then the "critical" droplet radius is $f_\mathrm{D} = f_\mathrm{S} \Rightarrow$ $R_\mathrm{c} = \frac{L}{\pi}$ and the "critical" magnetisation is $M_\mathrm{D}(R = R_\mathrm{c}) \equiv$ $M_c = m_0 L^2 (1 - \frac{2}{\pi})$.

- The right plot gives a graphical interpretation of $f_{\mathrm{D}} = f_{\mathrm{S}}$.
- The function with the lowest value (free energy) determines the shape.

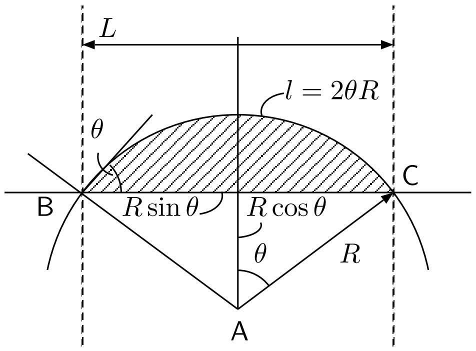


- Question: How do intermediate configurations look like?
  Answer: The droplet elongates along one axis.
  But: Minimal surface free energy ⇒ the shape is composed of spherical arcs (fixed total magnetisation).



4 How can this picture be numerically satisfied?

- Measuring the "hidden" free energy barriers: i.e. calculating the excess free energy at the worst point (maximal strechted droplet).



Sector and triangle:

$$A_{\mathrm{S}} = \theta R^2 \quad \text{and} \quad A_{\mathrm{T}} = R^2 \sin\theta\cos\theta\ .$$

Corresponding segment:

$$A_D = R^2(\theta - \sin\theta\cos\theta)$$

Conditions (maximal elongation and fixed magnetisation m):

$$2R\sin\theta = L \quad \text{and} \quad A_{\mathrm{D}} = L^2/\pi$$

gives:

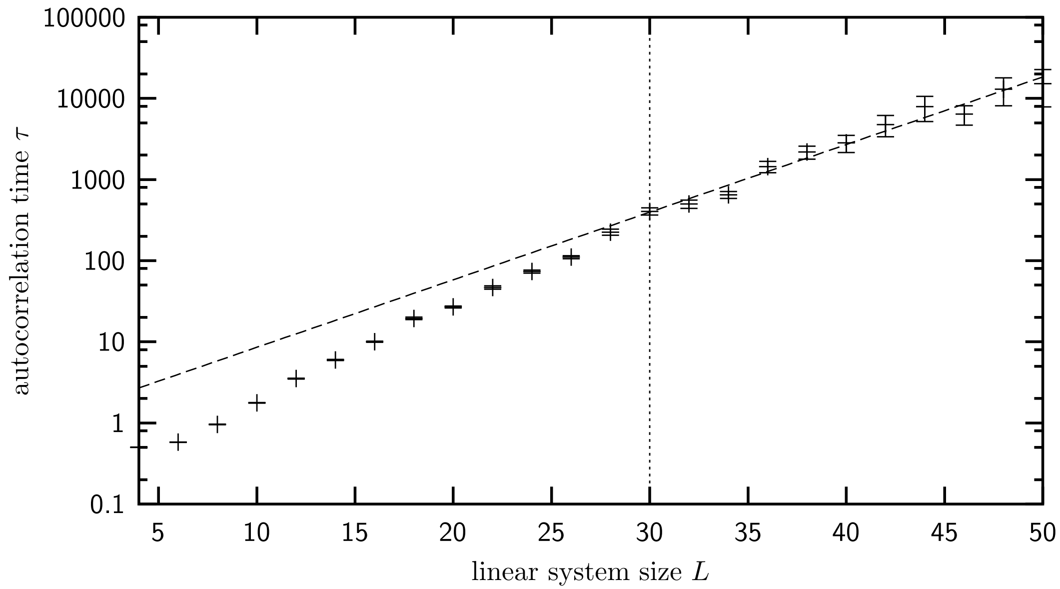
$$\boxed{\theta = \left(\frac{2}{\pi}\sin\theta + \cos\theta\right)\sin\theta}$$

Mathematica: $\theta = 0.860...$

Length of the boundary: $\partial A = 4\theta R = 2L\frac{\theta}{\sin\theta} \approx 1.13 \times 2L$

Difference between the boundary of a droplet $\partial A = 2L$ and strechted droplet is:

$$\Delta A = \left(\frac{\theta}{\sin\theta} - 1\right) 2L \approx 0.135 \times 2L \quad \text{or} \quad \tau \sim \exp(\underbrace{0.135}_{\alpha} \times 2\sigma\beta L)$$



The fitted range is:

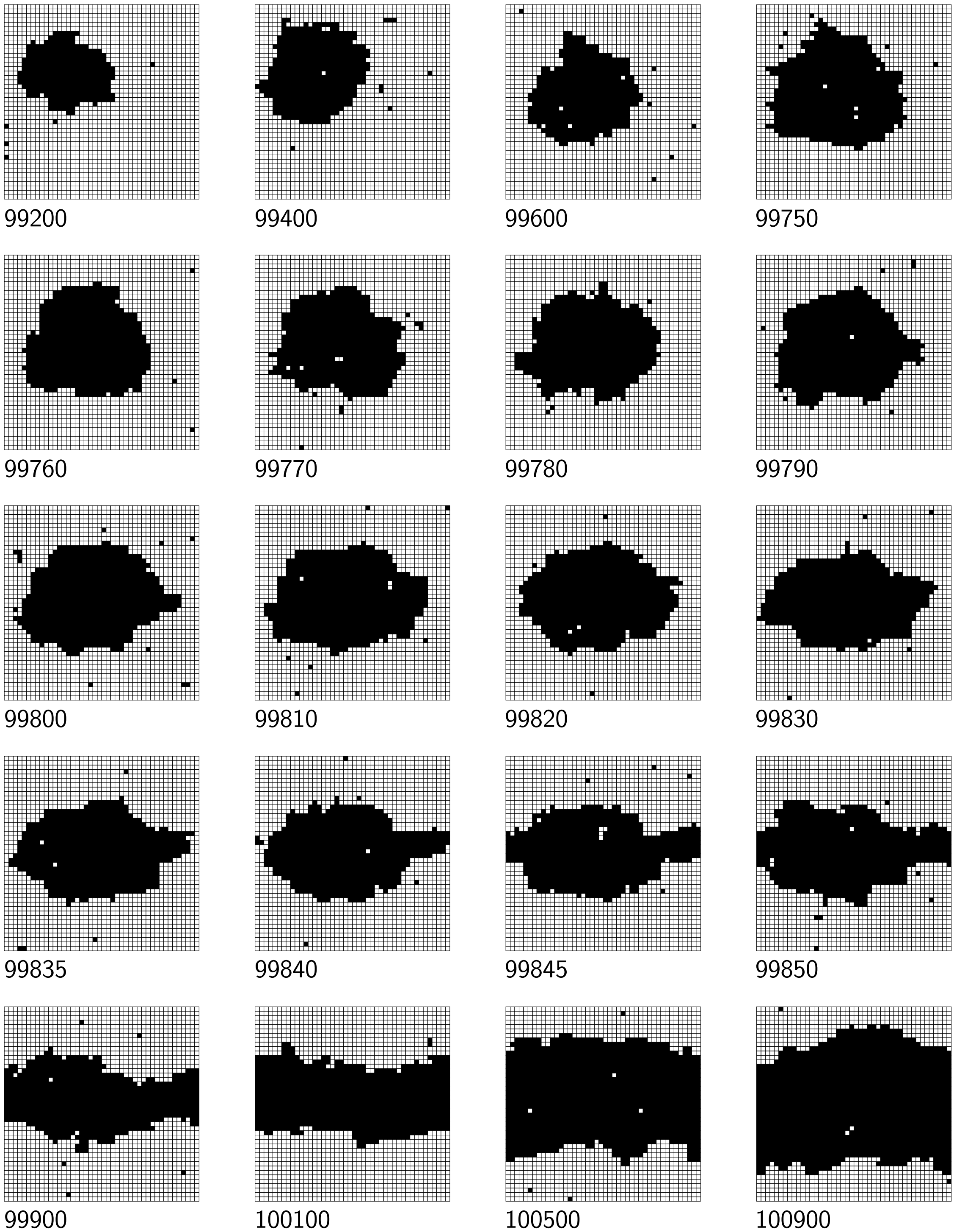
$L = 30$ to $L = 50$

giving:

$\alpha \approx 0.129 \pm 0.007$

But: very demanding simulation ($> 10^8$ MC sweeps for $L = 50$) and still large error bars!

- Checking the spin configurations visually:



Here: result of a 44×44 MuM simulation, i.e. magnetisation M is <u>not</u> fixed! (☞ animation).

- "Direct" measurement of the barrier size: i.e. classification of the configurations according to their geometrical shape.
  - Introduction of the anisotropy parameter:

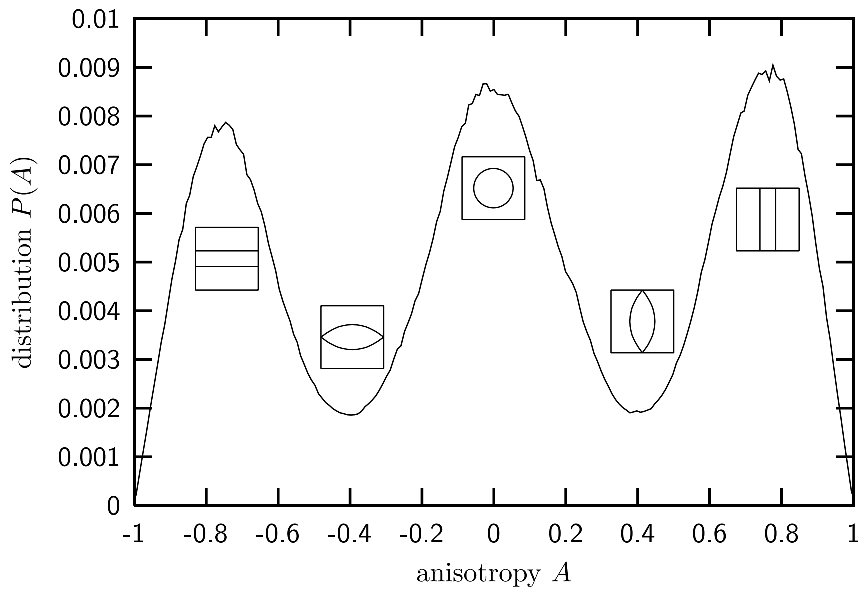
    $$\boxed{A \equiv \frac{s_x - s_y}{s_x + s_y}}$$

    where $s_x = |Y_{1,0}|$ and $s_y = |Y_{0,1}| \Rightarrow$ absolut values of the Fourier coefficients with modes $\vec{k}_x = (2\pi/L, 0)$ and $\vec{k}_y = (0, 2\pi/L)$.
  - Essentially:

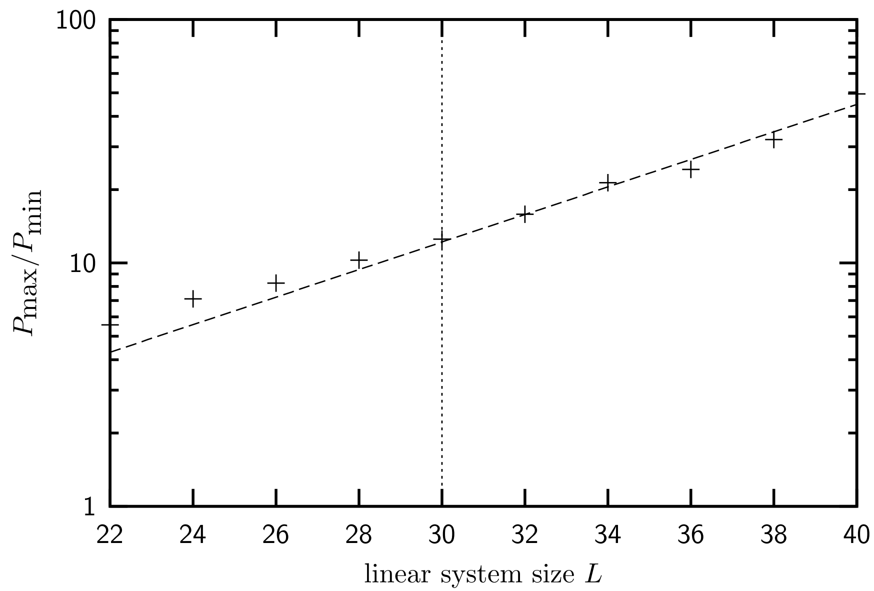
droplet:	$s_x = s_y > 0$	$\Rightarrow$	$A = 0$
strip:	$s_x > 0$ and $s_y = 0$	$\Rightarrow$	$A = +1$
	$s_x = 0$ and $s_y > 0$	$\Rightarrow$	$A = -1$

  - Simulation at a fixed magnetisation M_c where the peaks $P(A_\mathrm{D})$ and $P(A_\mathrm{S})$ have the same height.

- 20×20 MuA, $M =$ const. simulation, with $M = 116$ at a temperature $T = 1.5$.
- The symbols indicate the corresponding shapes.



- Linear fit to $\ln(P_{\text{max}}/P_{\text{min}})$ in the range $L = 30$ to $L = 40$.
- $\alpha = 1.30 \pm 0.01$

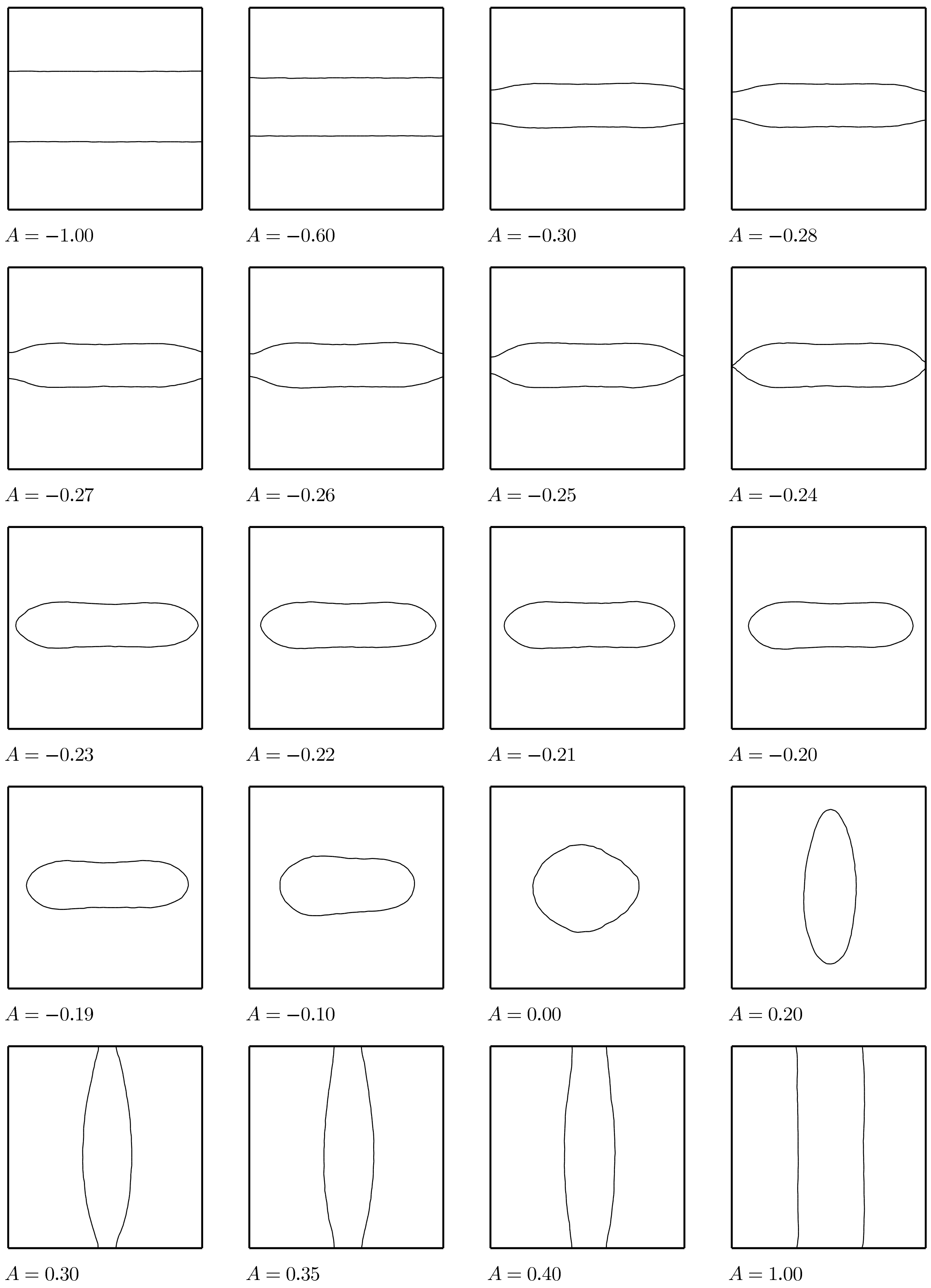


- Measurement of the equilibirum crystal shape: i.e. average spin configuration in dependence of the anisotropy parameter A.

  Technically:

  - Performing a MuA simulation to obtain weights $W(A)$.
  - Performing $M = \text{const.}$ (Kawasaki dynamics) + MuA simulation (using weights from previous simulation) and measuring:
    a) Center of mass of 2nd largest droplet ($\Rightarrow$ Hoshen-Koplelman algorithm)
    b) Anistropy
  - Shifting spin-configuration to have COM at $(L/2, L/2)$
  - Add spin-configuration according to $A \Rightarrow$ histogram $h(x, y, A)$

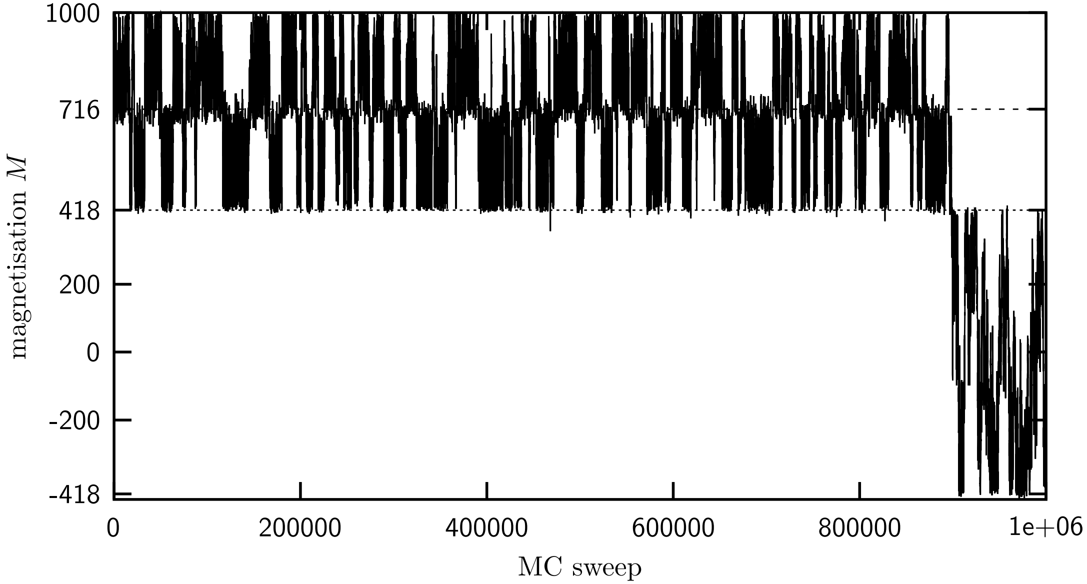
  Next page: results of the $M =$ const.-MuA-simulation on a 50×50 lattice at temperature $T = 2.0$ with 10^5 MC sweeps.



$A = -1.00$
$A = -0.60$
$A = -0.30$
$A = -0.28$
$A = -0.27$
$A = -0.26$
$A = -0.25$
$A = -0.24$
$A = -0.23$
$A = -0.22$
$A = -0.21$
$A = -0.20$
$A = -0.19$
$A = -0.10$
$A = 0.00$
$A = 0.20$
$A = 0.30$
$A = 0.35$
$A = 0.40$
$A = 1.00$

5 The three-dimensional case

- Closer look at the time series:

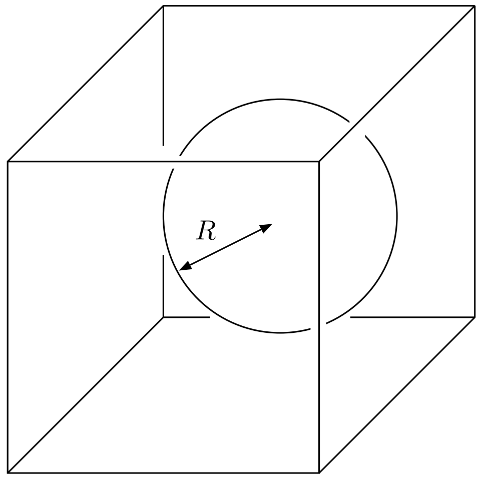


- Obviously there is a third configuration that is “stable” inbetween the sphere and the plane.

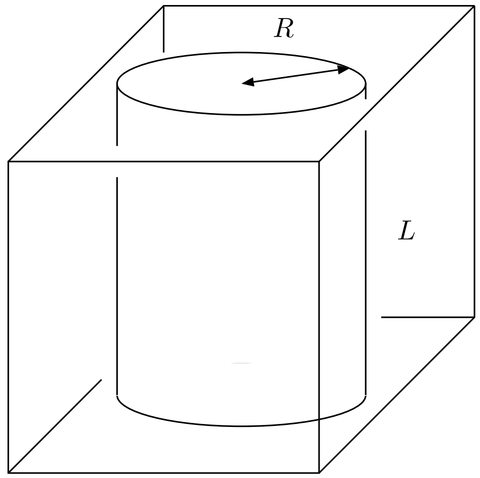
- Can this be understood theoretically?

- Again: the interface tension is isotropic and for all objects the same!

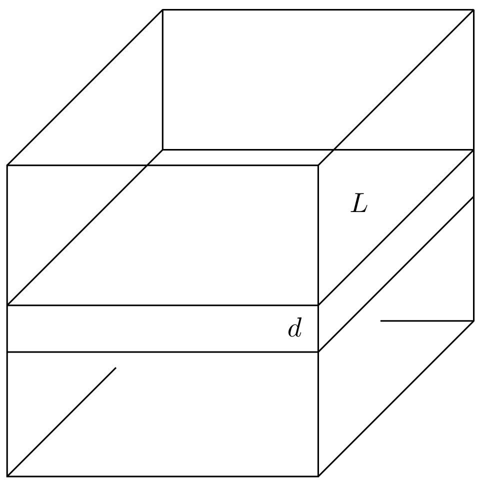
Sphere:



Cylinder:



Plane:



$$M_{\mathrm{Sp}} = m_0(L^3 - 2 \times \frac{4}{3}\pi R_{\mathrm{Sp}}^3)$$

$$M_{\mathrm{Cy}} = m_0(L^3 - 2\pi R_{\mathrm{Cy}}^2 L)$$

$$M_{\mathrm{Pl}} = m_0(L^2(L-d) - dL^2) = m_0(L^3 - 2dL^2)$$

$$f_{\mathrm{Sp}} = f_0 + 4\pi R_{Sp}^2 \sigma$$

$$f_{\mathrm{Cy}} = f_0 + 2\pi R_{Cy} L \sigma$$

$$f_{\mathrm{Pl}} = f_0 + 2L^2 \sigma$$

- Now, two transitions: sphere $\leftrightarrow$ cylinder and cylinder $\leftrightarrow$ plane.

Sphere $\leftrightarrow$ cylinder:

$$f_{\rm Sp} = f_{\rm Cy} \Rightarrow R_{\rm Sp,c} = \frac{L}{\sqrt{2\pi}}$$

Cylinder $\leftrightarrow$ plane:

$$f_{\rm Cy} = f_{\rm Pl} \Rightarrow R_{\rm Cy,c} = \frac{2R^2_{\rm Sp,c}}{L}$$

– Additional constrain: magnetisation at the transition point is equal:

$$M_{\rm Sp} = M_{\rm Cy} \Rightarrow R_{\rm Cy,c} = \frac{L}{3}.$$

– "Critical" magnetisation:

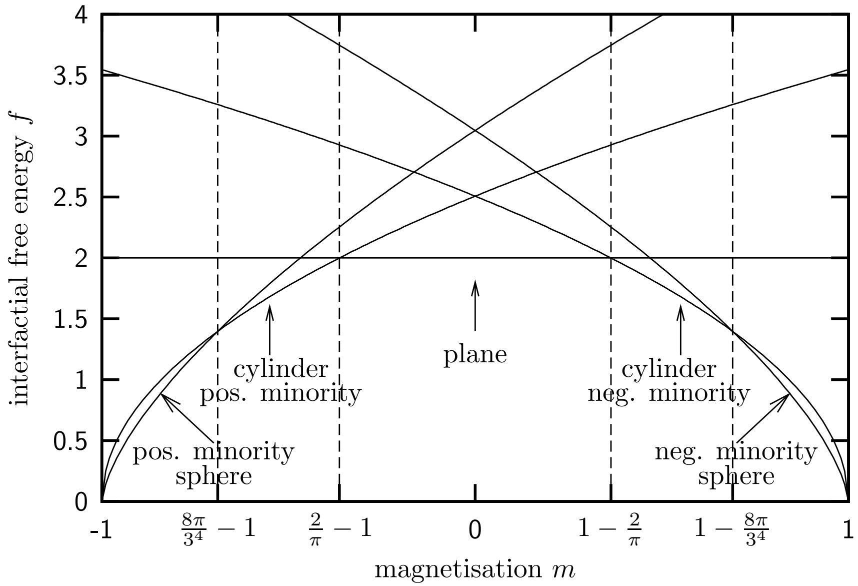
Sphere $\leftrightarrow$ cylinder:

$$M_{\rm Sp \leftrightarrow Cy} = m_0 L^3 (1 - \frac{8\pi}{3^4})$$

Cylinder $\leftrightarrow$ plane:

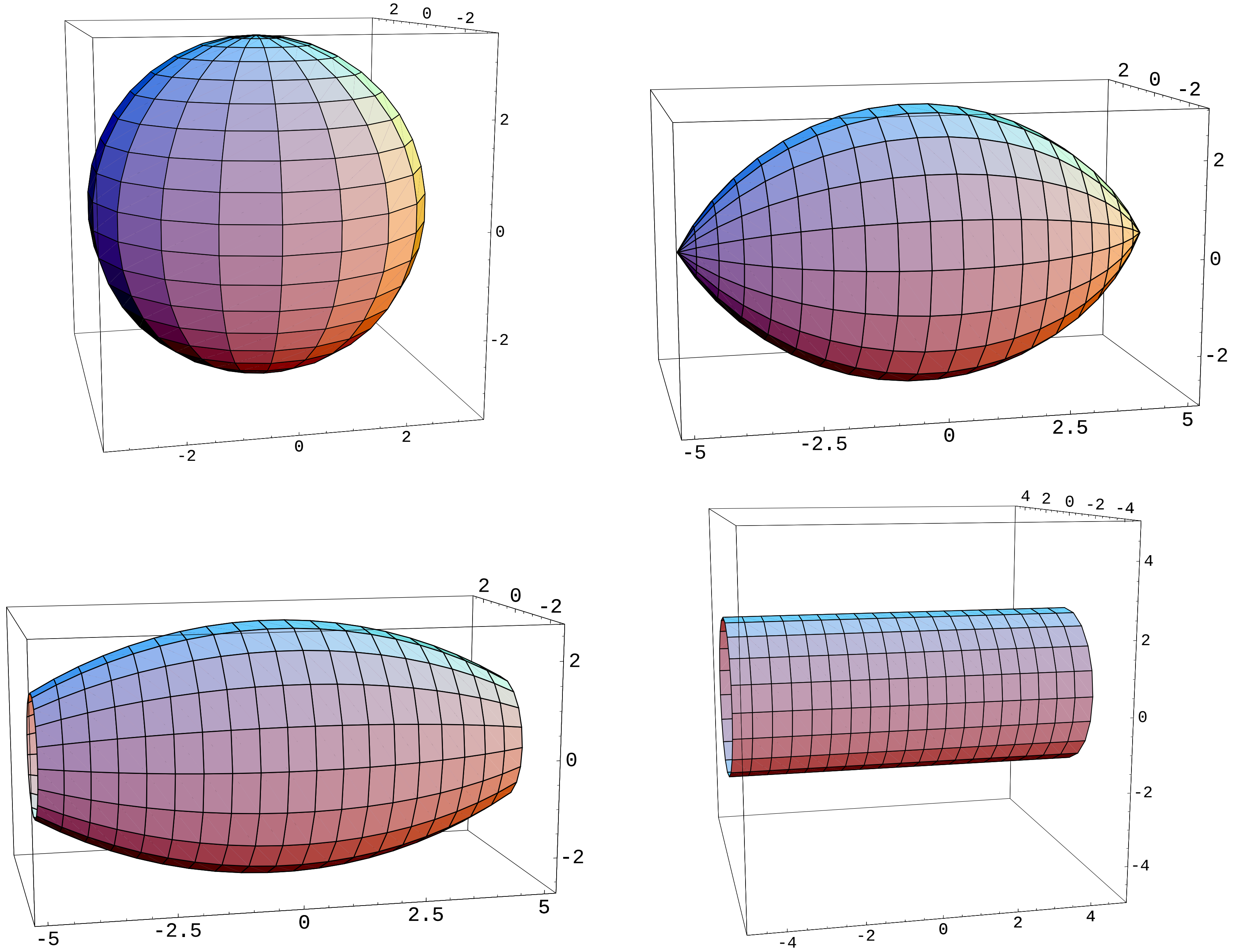
$$M_{\rm Sp \leftrightarrow Cy} = m_0 L^3 (1 - \frac{2}{\pi})$$

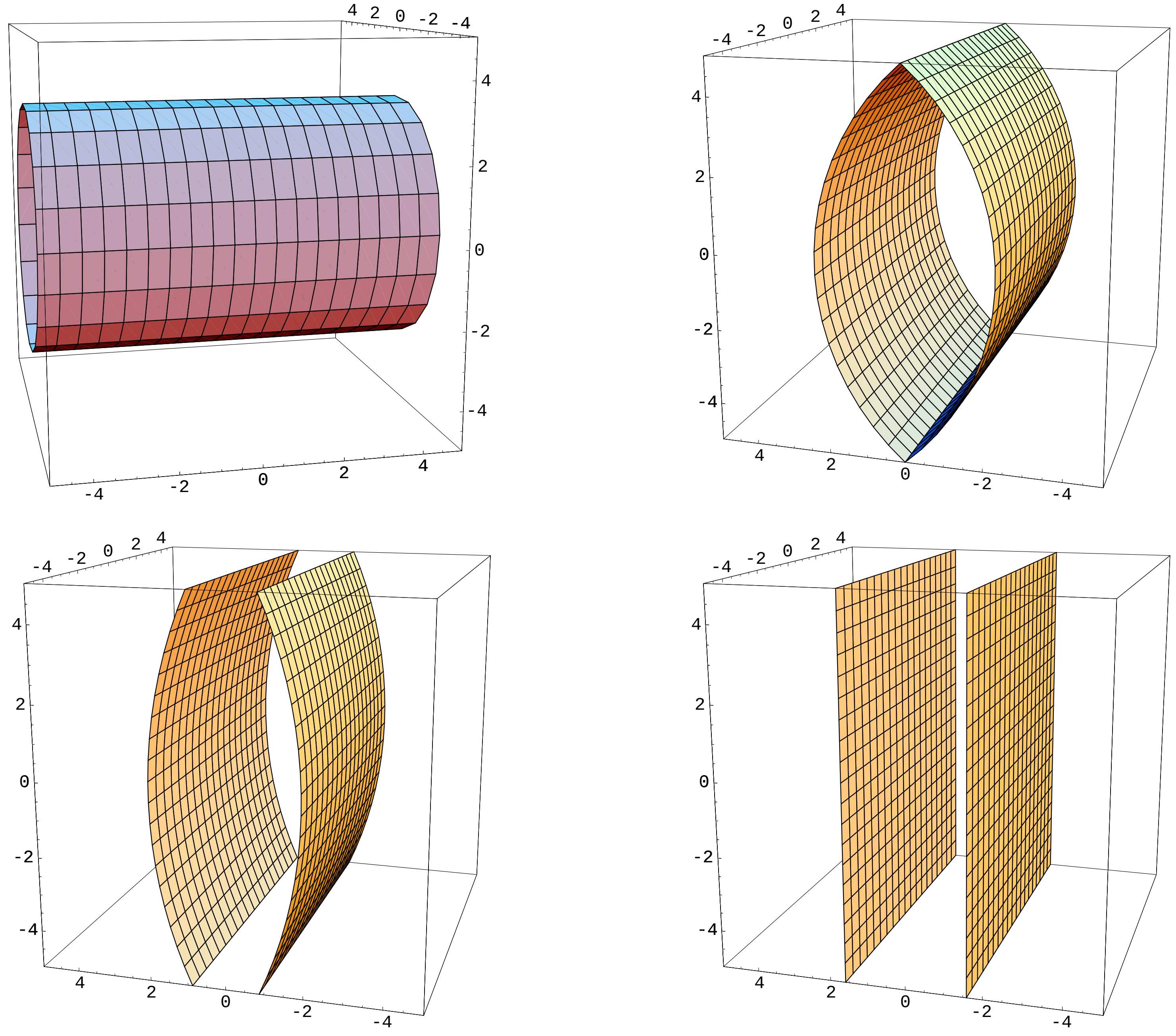
- The right plot gives a graphical interpretation of $f_{\mathrm{Sp}} = f_{\mathrm{Cy}}$ and $f_{\mathrm{Cy}} = f_{\mathrm{Pl}}$
- The function with the lowest value (free energy) determines the shape.



- Question (again): How do intermediate configurations look like?
  Answer (again):
  - The sphere elongates along one axis.
  - The cylinder elongates along one axis perpendicular to its main axis.

  But (again): Minimal surface free energy $\Rightarrow$ the shape is composed of spherical arcs (fixed total magnetisation).


2 0 -2
2
0
-2
-2 0 2
2 0 -2
2
0
-2
-5 -2.5 0 2.5 5
2 0 -2
2
0
-2
-5 -2.5 0 2.5 5
4 2 0 -2 -4
4
2
0
-2
-4
-4 -2 0 2 4


4 2 0 -2 -4
4
2
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-4 -2 0 2 4
-4 -2 0 2 4
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4 2 0 -2 -4
-4 -2 0 2 4
4
2
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4 2 0 -2 -4
-4 -2 0 2 4
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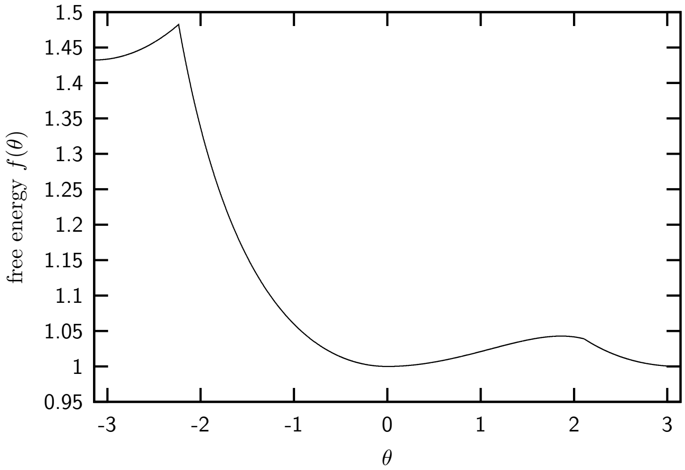
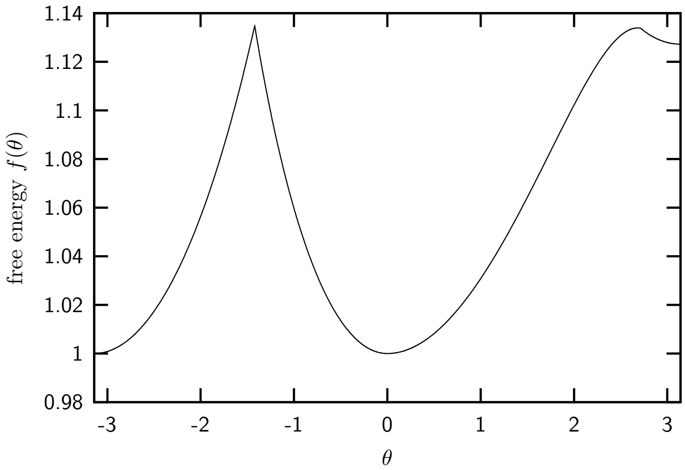
4 2 0 -2 -4

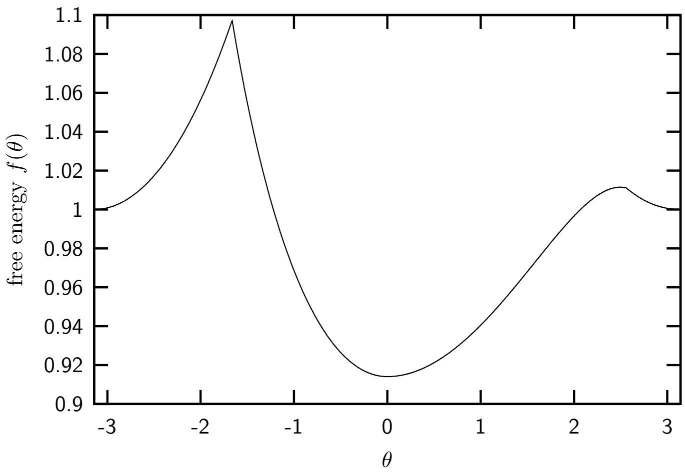
- Droplet ↔ cylinder:



- Cylinder ↔ plane:

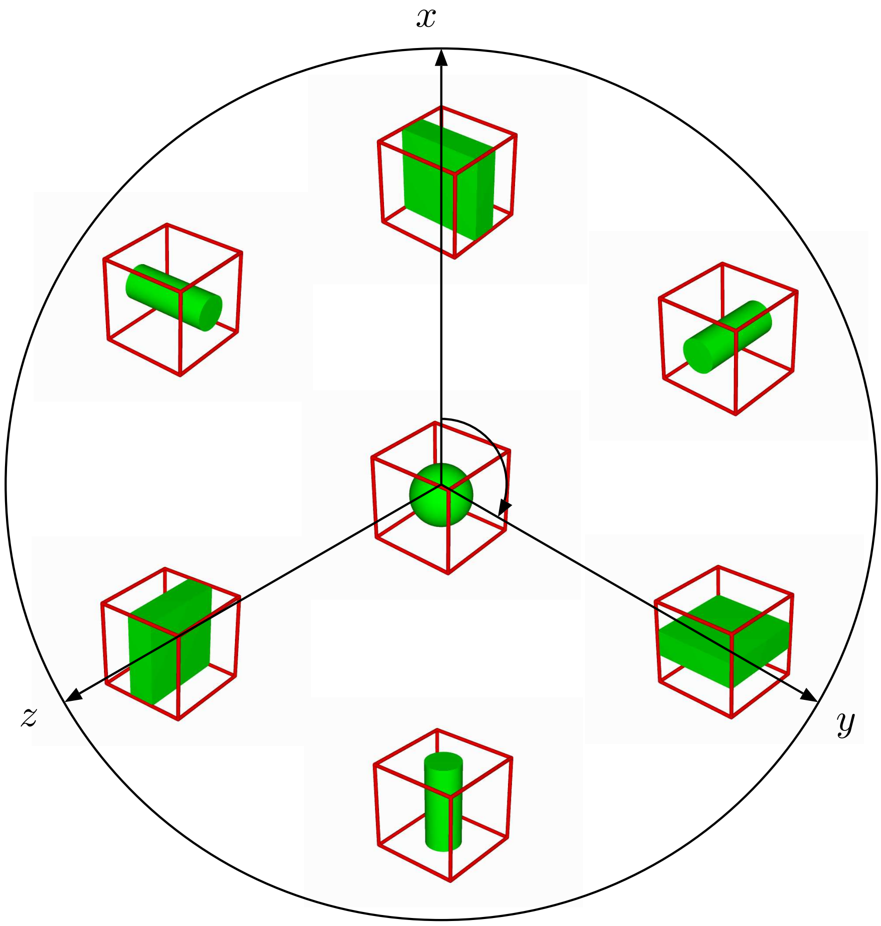


- Plane ↔ droplet:

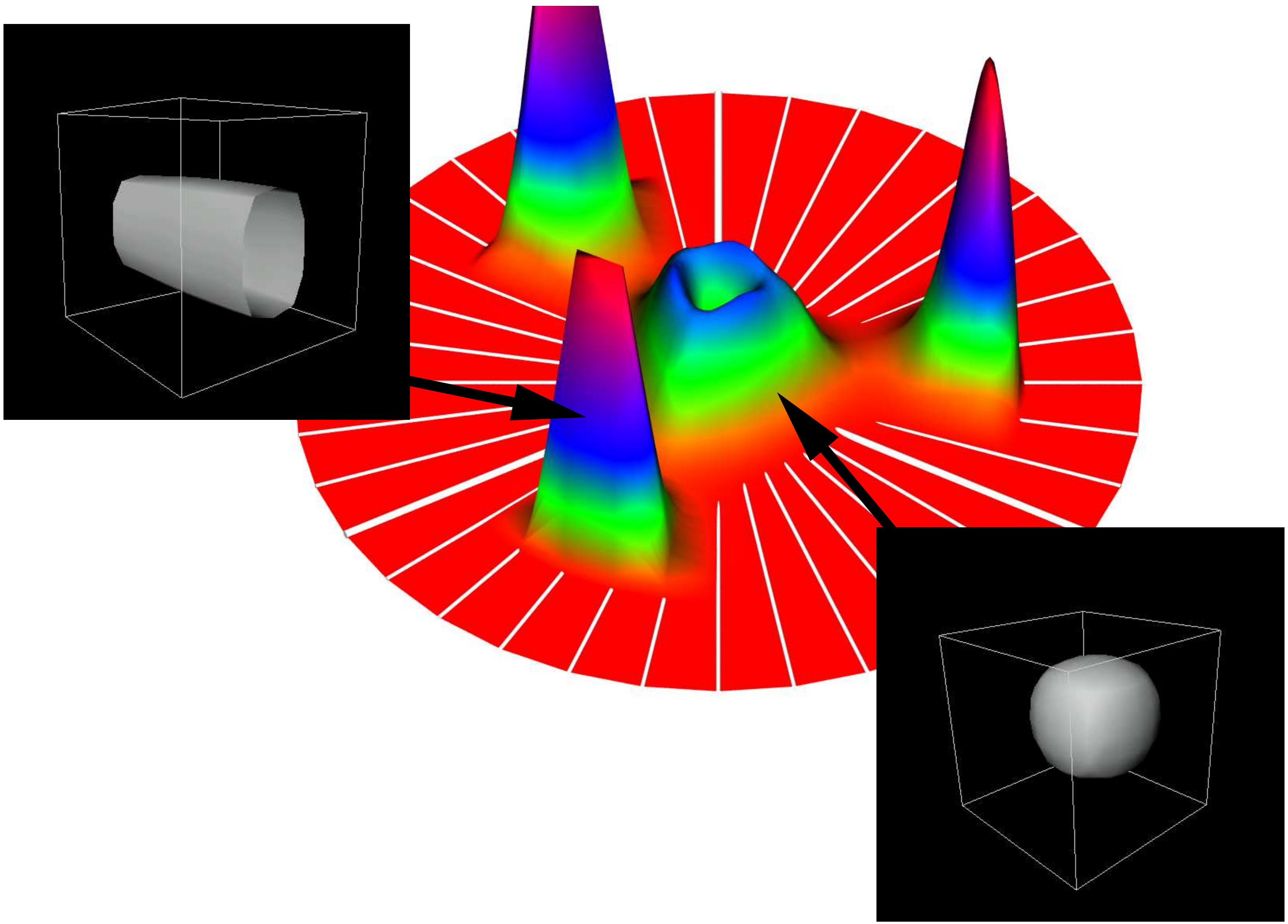


- 3D-Anisotropy parameter:

$$A_3 = \frac{s_x \hat{x} + s_y \hat{y} + s_z \hat{z}}{\sqrt{s_x^2 + s_y^2 + s_z^2}}$$



- Droplet-Cylinder transition:



- Cylinder-Slab transition: