

Monte Carlo Test of the Classical Theory for Heterogeneous Nucleation

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Classical nucleation theory

Homogeneous nucleation:

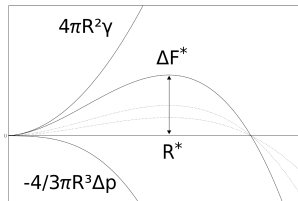
$$F_{hom} = -\frac{4\pi R^3}{3} \Delta p + 4\pi R^2 \gamma$$

$$\Delta F_{hom}^* = \frac{4\pi}{3} R^{*2} \gamma$$

Heterogeneous nucleation:

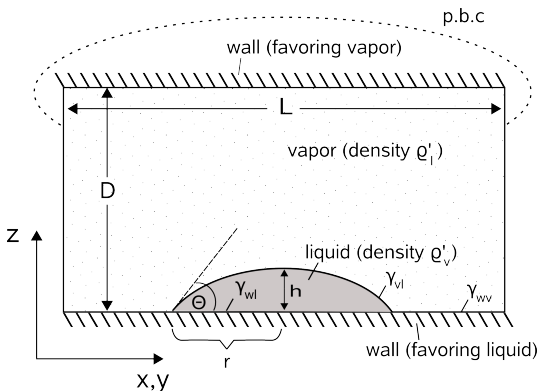
$$F_{het} = F_{hom} f(\theta)$$

$$f(\theta) = (1 - \cos \theta)^2 (2 + \cos \theta) / 4$$

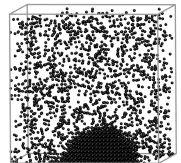
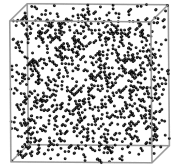
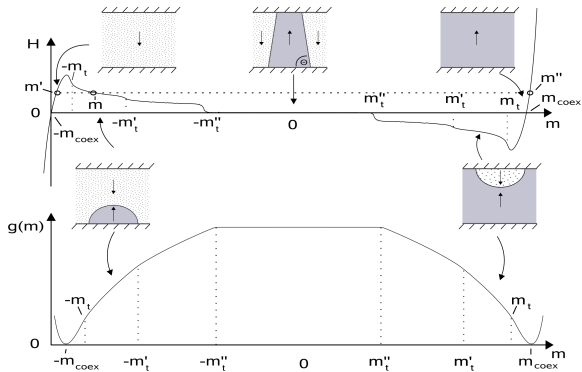


The model

- Magnetization is constant
- Metropolis step: $\downarrow\uparrow\rightleftharpoons\uparrow\downarrow$
- $H_D = -H_1$



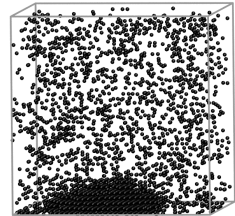
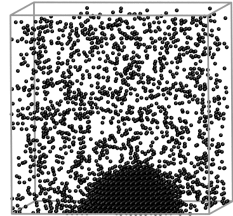
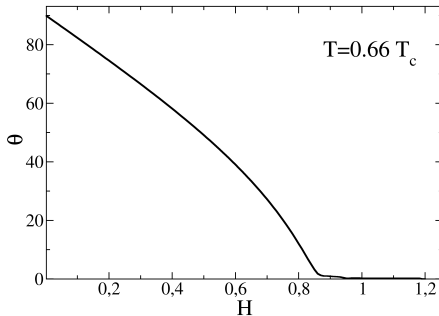
$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j - H_1 \sum_{z=1} \sigma_i - H_D \sum_{z=D} \sigma_i$$



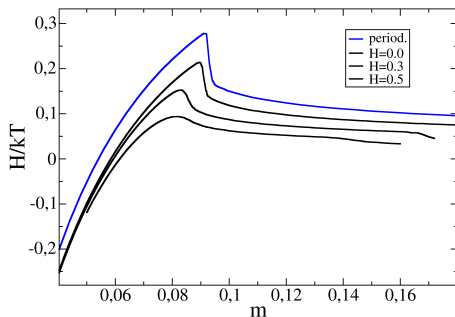
Measurement of the contact angle

Young Equation:

$$\cos \theta = \frac{\gamma_{wv} - \gamma_{wl}}{\gamma_{lv}} = \frac{\int_{-H_1}^{H_1} dH'_1 m_1}{\gamma_{lv}}$$



Measurement of the free energy



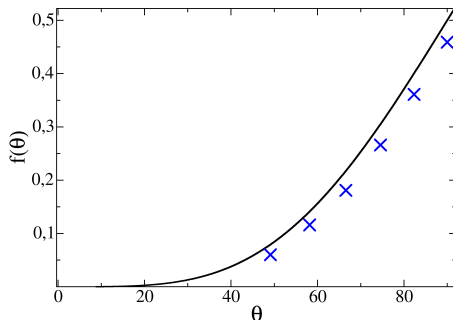
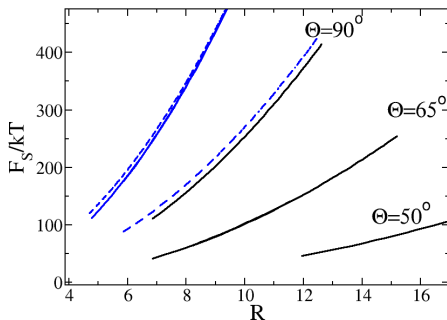
$$\begin{aligned}
 M &= m' V_v + m'' V_l \\
 &= m' (V - V_l) + m'' V_l \\
 V_l &= \frac{(m - m')}{(m'' - m')} V \quad (1) \\
 &= \frac{4}{3} \pi R^3 f(\theta) \\
 \Rightarrow R &= \sqrt[3]{\frac{3 V_l}{4 \pi f(\theta)}}
 \end{aligned}$$

$$F_{surf} = V \int_{m_1}^{m_2} dm H$$

The surface free energy of the droplet

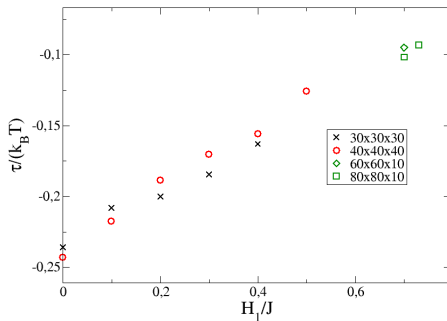
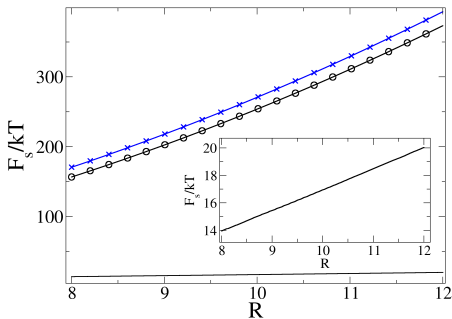
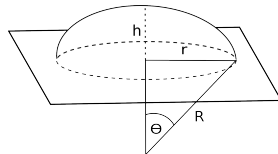
$$F_{het} = F_{hom} f(\theta)$$

$$f(\theta) = (1 - \cos \theta)^2 (2 + \cos \theta) / 4$$

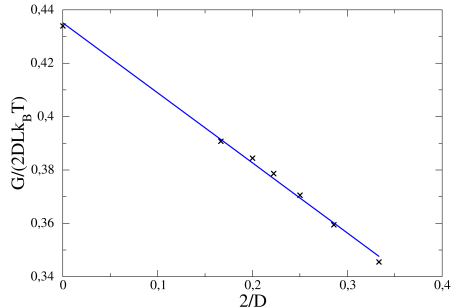
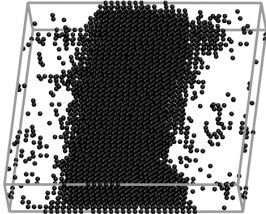


The line tension

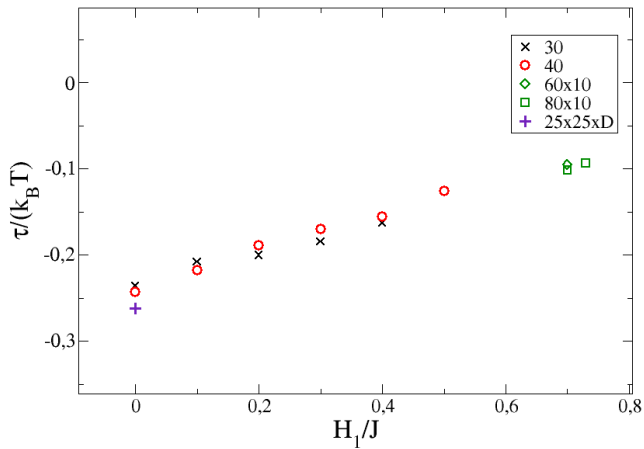
$$F_{het} = \gamma \cdot A + \tau \cdot s$$



The slab state



$$\begin{aligned}\Delta G &= 2DL\gamma_{lv} + 4L\tau \\ &= 2DL\left(\gamma_{lv} + \frac{2}{D}\tau\right)\end{aligned}$$



Thank you for your attention !