

Lattice Gas models including water-surface interactions

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1 Model

We study the interaction of water and surfaces using Monte Carlo simulations in the grand canonical (GC) ensemble. The lattice-gas is a simplified model where water is represented as two-dimensional lattice with a spacing given by the average distance between water molecules, l . Each lattice site can be either occupied or empty. The GC Hamiltonian in the presence of surfaces is given by:

$$H = -\epsilon \sum_{\langle i,j \rangle} c_i c_j - b_s \sum_{i \in \mathcal{S}} c_i - \mu \sum_i c_i \quad (1)$$

where c_i is the occupancy state of lattice site i ($c = 1$ for a occupied site and $c = 0$ for empty site) and ϵ is the attractive energy between water molecules. The chemical potential is given by μ and b_s is the interaction energy between water and surfaces, where $b_s > 0$ for hydrophylic surfaces and $b_s < 0$ for hydrophobic surfaces. The chemical potential is given by $\mu = \mu_c + k_B T \log s$ where s is the water saturation (relative humidity) and the critical chemical potential is a known value.

After appropriate algebraic manipulation, Equation 1 can be modified to map with the Ising model, where the spins are in states ± 1 , resulting in

$$H = -\epsilon \sum_{\langle i,j \rangle} s_i s_j + \frac{2\epsilon + \mu}{2} \sum_i s_i - \frac{b}{2} \sum_{i \in \mathcal{S}} (1 - s_i), \quad (2)$$

where ϵ is analogous to the coupling constant and the term $\frac{2\epsilon + \mu}{2}$ is analogous to the magnetic field. In that form, $s_i = -1$ indicates an occupied lattice site nad $s_i = 1$ is an empty site.

We use periodic boundary conditions and a von Neumann neighborhood for the interaction between water-water and water-surface. Minimisation proceeds by randomly selecting lattice locations and comparing the energy change following the Metropolis criterion.

Parameter	Value	References
General parameters		
Temperature, T	298 K	
Water-water, ϵ	3	
AFM tip simulations		
Number lattice sites horizontal, w	100	
Number lattice sites vertical, h	100	
Tip radius R	10 nm	
Tip surface distance y_0	0.5 l	
Relative humidity, s	0.30-0.65	
Icosahedral virus simulations		
Virus radius, R	25 nm	
Virus shell thickness, t	3 nm	

Table 1: Simulation parameters.

General and simulation specific parameters

2 Meniscus between surface and AFM tips

We consider the AFM tip as the values above the parabola given by $y(x) = ax^2 + y_0$, where y_0 is the distance to the surface and $a = \frac{1}{2R}$, with R the desired radius of the tip. The later is determined from the second derivative of $y(x)|_{x=0}$.

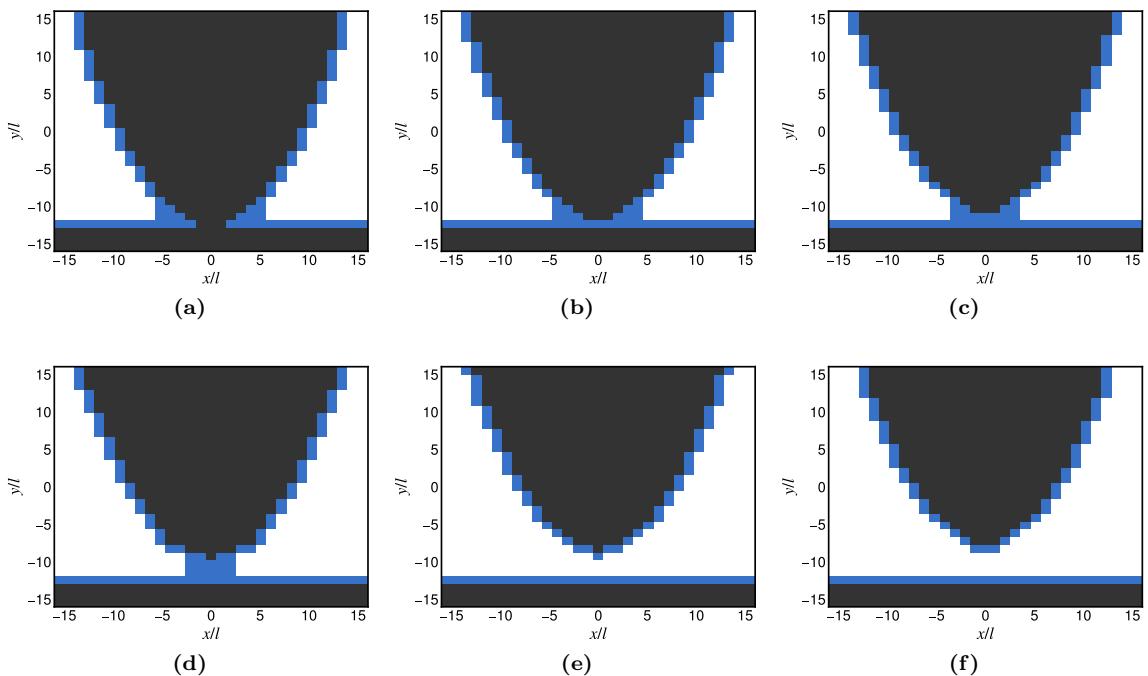


Figure 1: Water meniscus depepending on the distance to surface

Retraction from $y_0 = 0$ to $y_0 = 5$ in steps of l ($y_0 = 0, l, 2l, 3l, 4l, 5l$). The blue areas corresponds to regions with a probability of occupancy $n > 0.75$ obtained from 2000 Monte Carlo steps equilibration. Saturation $s = 0.30$.

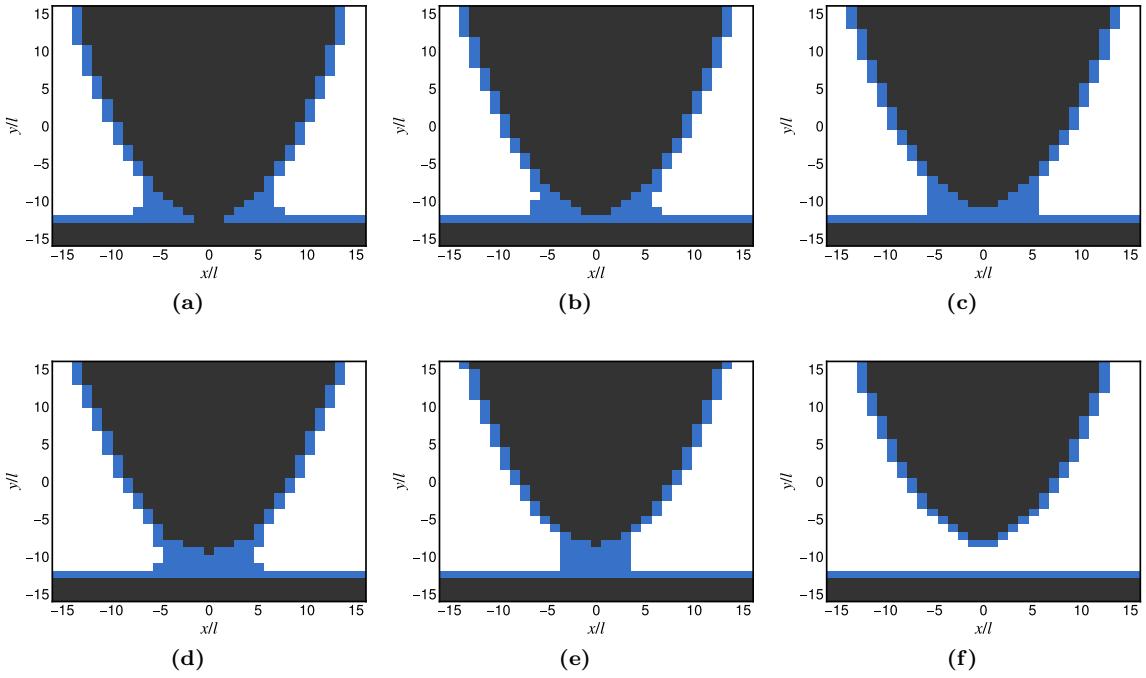


Figure 2: Water meniscus depending on the distance to surface

Retraction from $y_0 = 0$ to $y_0 = 5$ in steps of l ($y_0 = 0, l, 2l, 3l, 4l, 5l$). The blue areas corresponds to regions with a probability of occupancy $n > 0.75$ obtained from 2000 Monte Carlo steps equilibration. Saturation $s = 0.50$.

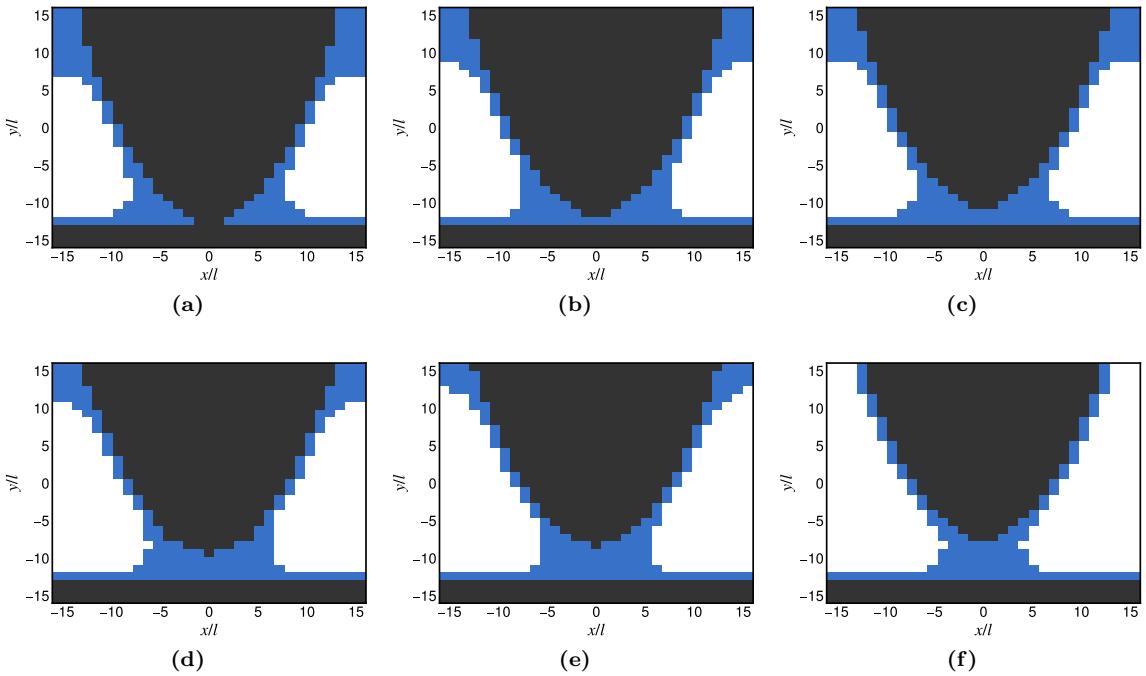


Figure 3: Water meniscus depending on the distance to surface

Retraction from $y_0 = 0$ to $y_0 = 5$ in steps of l ($y_0 = 0, l, 2l, 3l, 4l, 5l$). The blue areas corresponds to regions with a probability of occupancy $n > 0.75$ obtained from 2000 Monte Carlo steps equilibration. Saturation $s = 0.65$. Note the artifact on the upper part due to the limited size of the mesh in the horizontal direction.

3 Icsaohedral viruses

We draw the icosahedron from the polar function

$$r = R(1 + A \sin 6\theta), \quad (3)$$

where R is the radius of the icosahedron, A is a shape parameter set to $A = 0.06$ and θ spans a range between θ_0 and 2π . A virus with a cavity can be draw by considering $\theta_0 > 0$. Viruses with multiple cavities can be constructed by restricting the domain of θ .

References

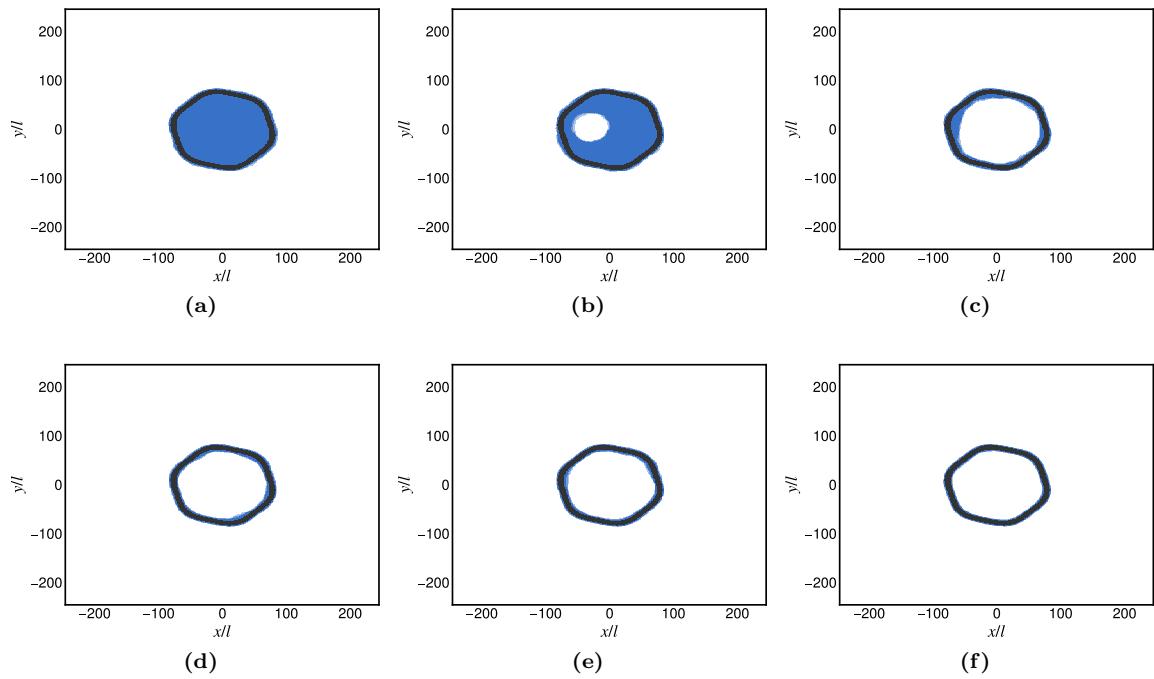


Figure 4: Dessication of icosahedral virus

Retraction from $y_0 = 0$ to $y_0 = 5$ in steps of l ($y_0 = 0, l, 2l, 3l, 4l, 5l$). The blue areas corresponds to regions with a probability of occupancy $n > 0.75$ obtained from 2000 Monte Carlo steps equilibration. Saturation $s = 0.50$.