# 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 cannonical ensemble. The lattice-gas is a simplified model where water is reppresented 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 Hamiltonian in the presence of surfaces is given by:

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

where $c_i$ is the occupancy state of lattice site $i$ ($c = 1$ for a occupied site and $c = 0$ for empty site) and $\epsilon$ is the attractive energy between water molecules. The chemical potential is given by $\mu$ 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 humidty) and the critical chemical potential is a known value.

After appropiate algebraic manipulation, Equation 1 can be modified to map with the Ising model, where the spins are in states $\pm 1$, resulting in

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

where $\epsilon$ 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.

| Parameter | Value |
|---|---|
| **General parameters** | |
| Temperature, $T$ | 298 K |
| Water-water, $\epsilon$ | 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, $R$ | 50 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.

Minimisation proceeds by randomly selecting lattice locations and comparing the energy change following the Metropolis criterion.
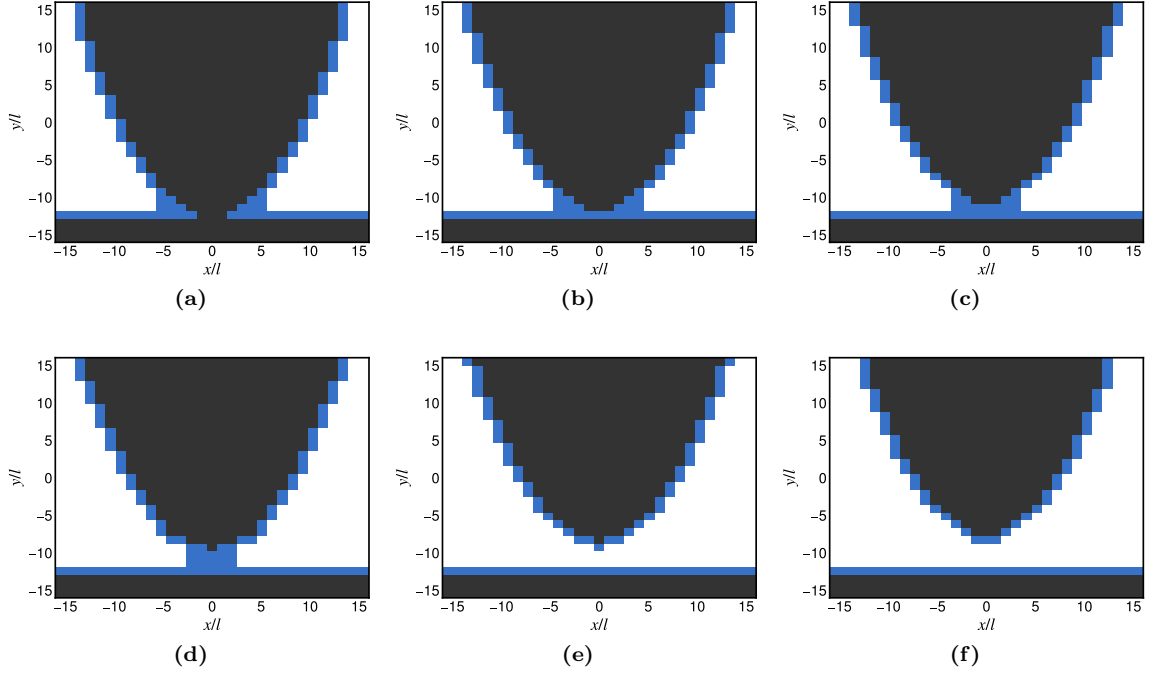


**Figure 1:** Water meniscus depeending on the distance to surface
Retraction from $y_0 = 0$ to $y_0 = 5$ in steps of $l$ ($y_0 = 0, l, 2l, 3l, 4l, 5l$). The blue areas corresponds to regions with a probability of occupancy $n > 0.75$ obtained from 2000 Monte Carlo steps equilibration. Saturation $s = 0.30$.
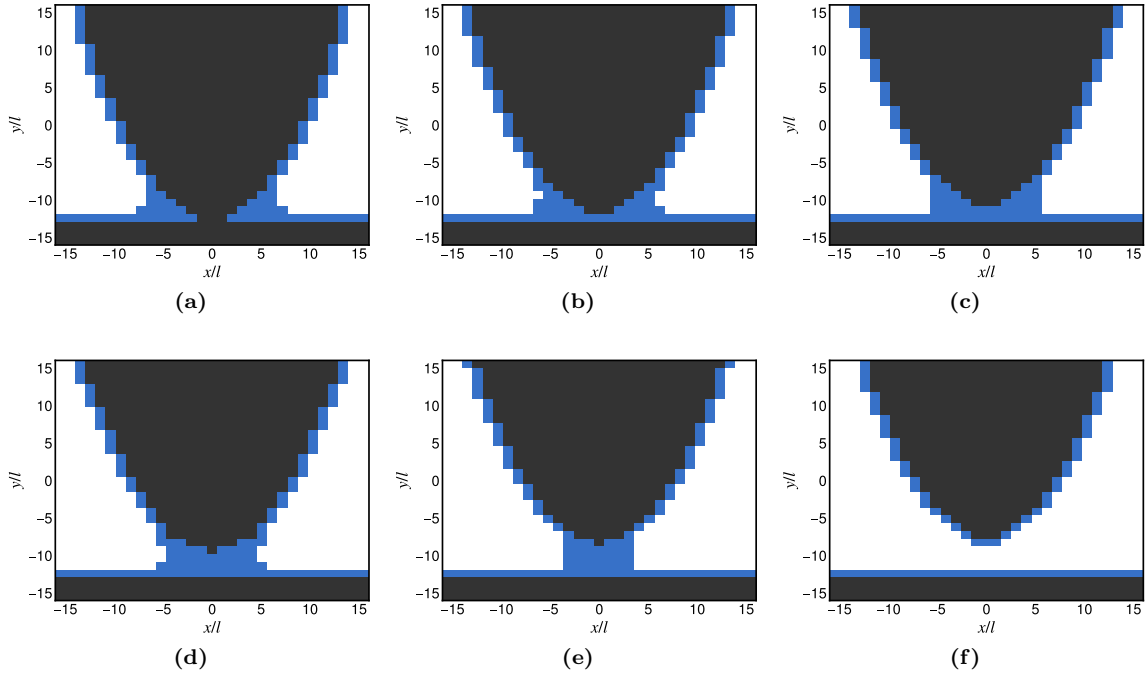
**Figure 2:** Water meniscus depepending on the distance to surface

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 $s = 0.50$.
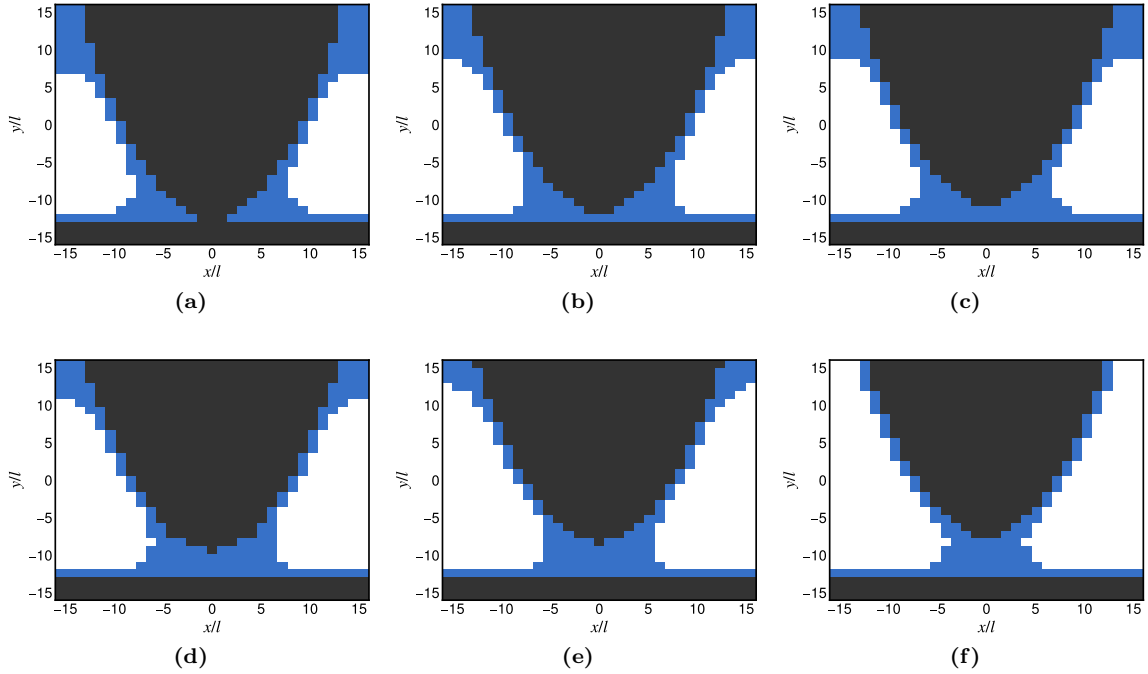


**Figure 3:** Water meniscus depepending on the distance to surface

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 $s = 0.65$. Note the artifact on the upper part due to the limited sie of the mesh in the horiontal direction.

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# 3   Icsaohedral viruses

References