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Computational Soft Matter Physics

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Problem 8: Interface Fluctuations

The interface between two coexisting phases can be described for temperatures well below the critical point, in the Monge representation, by a height field $h(\mathbf{r})$, which measures the deviations of the interface position from a planar reference state. Here, $\mathbf{r}$ is a two-dimensional coordinate in the reference plane. Since this model neglects interface configurations with overhangs, it is sometimes called "solid-on-solid" (SOS) model.

To make the SOS model amenable to computer simulations, it is discretized in the lateral directions on a $N \times N$ square lattice. Each height variable h_i is a real number. The interface fluctuations are controlled by the surface tension σ, with an energy $\mathcal{H}$ given by

$$\mathcal{H} = -\sum_{<ij>} \sigma (h_i - h_j)^2 \tag{1}$$

where $< ij >$ indicates nearest-neighbor pairs. To avoid boundary effects, periodic boundary conditions are employed.

In the Monte Carlo steps, h_i is updated by a small increments, which are chosen from a uniform distribution in $[-\Delta h, \Delta h]$. Δh is determined by the requirement that approximately 50% of update attempts are accepted.

The interface width is given by

$$w = \left\langle N^{-1} \sum_i (h_i - \bar{h})^2 \right\rangle^{1/2} \tag{2}$$

where $\bar{h} = N^{-1} \sum_j h_j$ is the "center of mass" of each configuration.

(a) For fixed systems size $N = 20$, calculate w as a function of surface tension for $\sigma/k_BT = 0.25, 0.5, 1.0, 2.0, 5.0, 10.0$. Plot w as a function of σ/k_BT and extract the functional dependence.

(b) For fixed tension $\sigma/k_BT = 1.0$, determine the dependence of w on the system size for $N = 5, 10, 20, 40, 80$. Show that the numerical results are consistent with a logarithmic dependence on system size.

(c) For an interface close to a wall, which is pushed "gently" to the wall by a gravitational field, is described by the additional potential

$$\mathcal{H}_g = -\sum_i \rho g h_i \tag{3}$$

for $h_i > 0$, and $\mathcal{H}_g \to \infty$ for $h_i \leq 0$, where ρ is a mass density and g the gravitational force constant. Calculate the average wall separation $\bar{h}$ as a function of ρg for small surface tensions σ. iOn the basis of the simulation results, can you guess the functional dependence of $\bar{h}$ on ρg?

(d) A variant of the SOS model for interfaces between crystalline solids and liquids uses integer height variables $h_i \in \{..., -2, -1, 0, +1, +2, ...\}$. Use the increments ± 1 for the updates of the height variables. Calculate again w as a function of σ/k_BT for $N = 40$. How do the results differ from the case of continuous height variables?