Effective forces induced by fluctuating interface: exact results.

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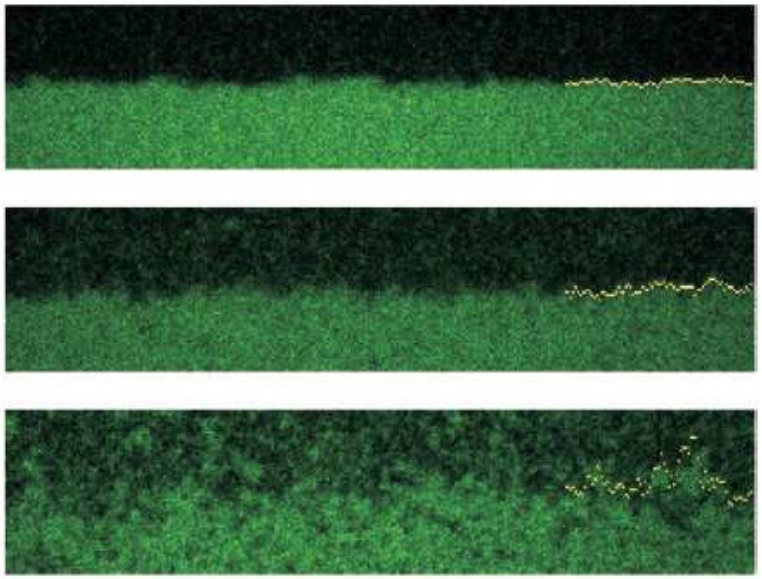
Douglas Abraham and Fabian Essler, University of Oxford,

Phys. Rev. Lett. **98**, *170602 (2007)*.

Capillary waves

- forces induced by fluctuations, both thermal and quantal, are ubiquitous in nature: from biophysics to cosmology $\longrightarrow$ Casimir forces
- thermal fluctuations of the interface above the roughening transition

D.G.A.L. Aarts, M. Schmidt, and H.N.W. Lekkerkerker, Science **304**, 847 (2004)

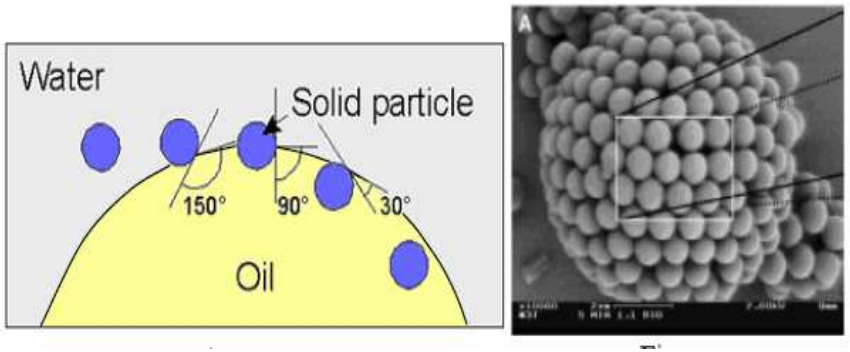


- geometric limitation of the configuration of the interface manifests itself in a long range attraction

physical systems

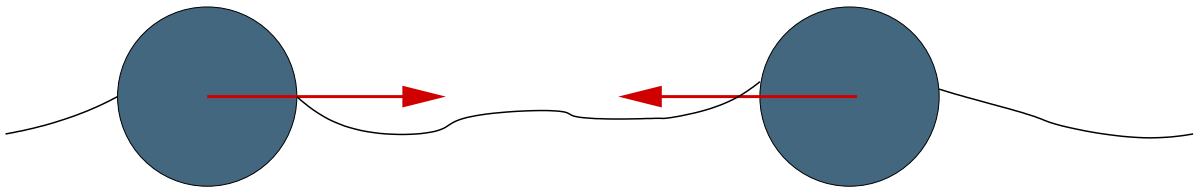
- colloidal particles trapped at the liquid-liquid or liquid-vapour interface at coexistence by chemicophysical forces

Pickering emulsions:



- Janus sphere - bifunctional particle with different wetting properties on two hemispheres

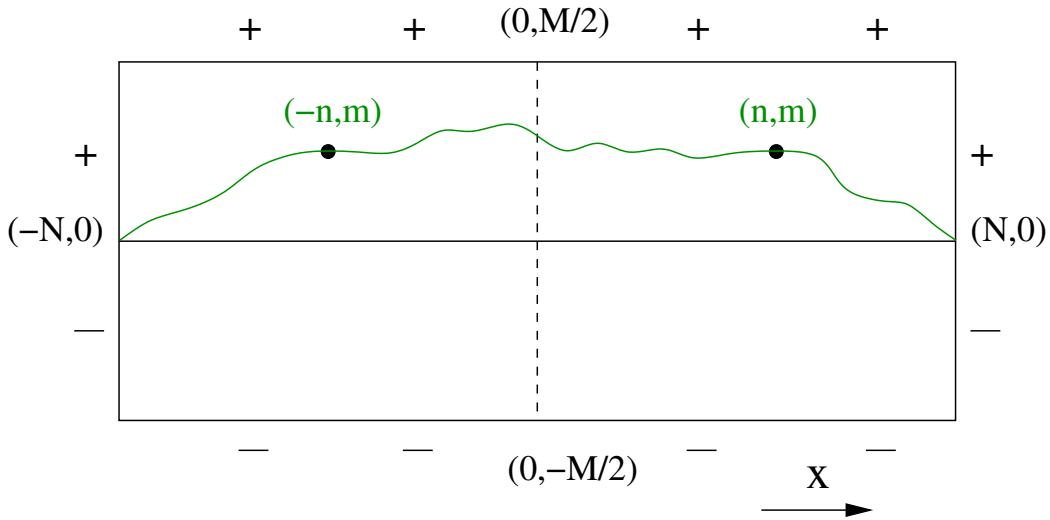
- colloids are spatially fixed at the interface and the contact lines are pinned, they restrict the motion of the interface strongly. The phase space restriction implies:



- what is the nature of the effective forces between colloidal particles at the interface?
- effective forces induced by capillary fluctuations of the interface?

$d = 2$ Ising model

$$\mathcal{H} = -K_1 \sum_{i,j} \sigma_{i,j}\sigma_{i+1,j} - K_2 \sum_{i,j} \sigma_{i,j}\sigma_{i,j+1}$$



incremental free energy of an interface resulting from pinning:

$$\beta f^{\times}(n) = -\lim_{N,M\to\infty} \ln \frac{Z^{\times}(n|N,M)}{Z(N,M)}$$

method

- column-to-column transfer matrix

$$V(|\sigma_i\rangle_l, |\sigma_i\rangle_m) = e^{-\beta E(|\sigma_i\rangle_l, |\sigma_i\rangle_m)}; \quad |\sigma_i\rangle = |\uparrow\rangle, |\downarrow\rangle$$

- partition function (periodic boundary conditions in y-direction)

$$Z(N, M) = Tr(V^N) = \sum_j \Lambda_j^N;$$

$$\lim_{N\to\infty} \frac{1}{N} \ln Z(N, M) = \ln(max\Lambda_j)$$

- 'domain wall state method' - achieves localization of the interface up to the bulk correlation length

Diagonalization of the TM

- mapping to a theory of free fermions $\rightarrow$; reduction 2^M down to $2M$

$$V = \exp[-\frac{1}{2}\sum_{k=1}^{M}\gamma(k)(2X_k^\dagger X_k - I)].$$

- eigenvectors of V:

'vacuum' $|\Phi\rangle$ $X_l|\Phi\rangle = 0$ for all l

$$\Lambda_0 = \exp\left(+\frac{1}{2}\sum_k \gamma(k)\right), \quad \cosh\gamma(k) = \cosh 2K \cosh 2K^* - \cos k$$

'excited states' $X_{l_1}^\dagger \ldots X_{l_j}^\dagger|\Phi\rangle$

- periodic BC: $e^{iMk} = \pm 1$

'Domain-wall state'

- $|k\rangle = X_k^\dagger|\Phi\rangle$ (domain walls) are associated with a wavenumber
- local one-particle states $|j\rangle$, which would be associated to a position j

$$|m\rangle = M^{-1/2}\sum_k \exp -ik(m+1/2)\ X^\dagger(k)|\Phi\rangle$$

- $|m\rangle$ localises the interface up to the bulk correlation length

$$Z^\times(n|N,M) = \sum_m \langle 0|V^{N-m}|m\rangle \times \langle m|V^{2n}|m\rangle\langle m|V^{N-n}|0\rangle$$

Excess free energy

$$\beta\ f^{\times}(n) = -\log\left[\int_0^{2\pi} \frac{d\omega}{2\pi} e^{-2n[\gamma(\omega)-\gamma(0)]}\right], \quad N, M \to \infty$$

- $\gamma(0) \sim \xi^{-1}$

  The asymptotics for large n of this are determined by the Laplace method

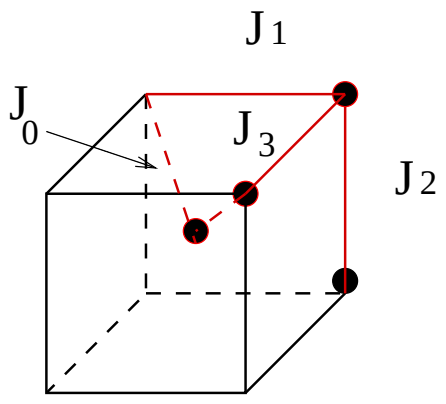
$$\beta\ f^{\times} \sim \log\sqrt{2\pi\gamma^{(2)}(0)r/a_0} + \mathcal{O}(1),$$

- $r = 2na_0$, valid for $n\gamma^{(2)}(0) \gg 1$, i.e., $r \gg a_0/\gamma^{(2)}(0)$, $1/\gamma^{(2)}(0)$ is the interface stiffness, a_0 the lattice constant

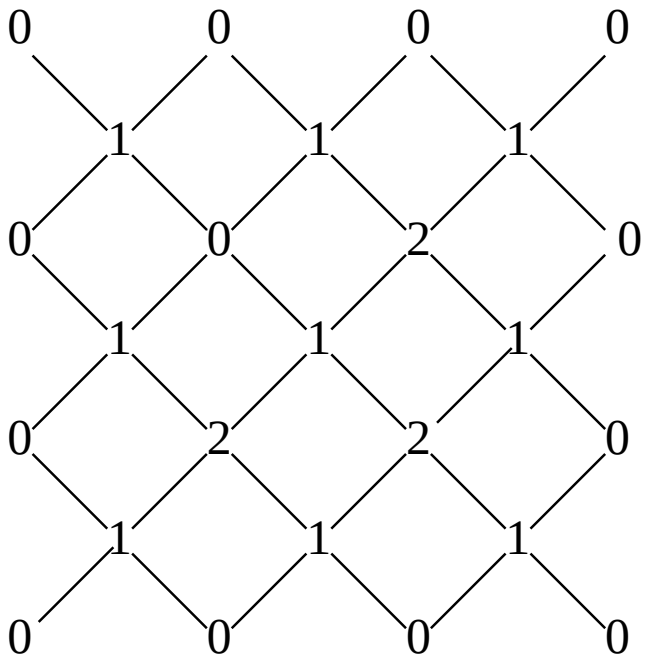
$$\mathcal{F}(r) \sim -\frac{kT}{2}\frac{1}{r}$$

$d = 3$

the van Beijeren BCSOS model (1977)



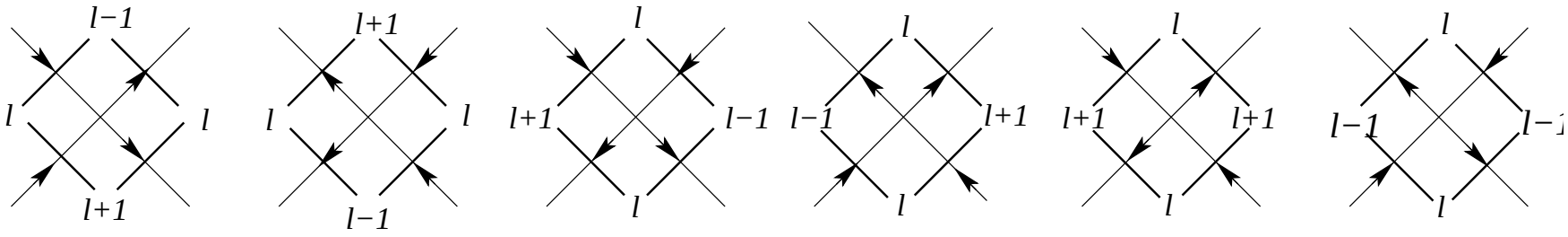
$J_1 = J_3 = J$



Proceeding in the $(1,1)$ direction, the height difference at a separation $r = 2na_0$ for integer n is $\delta h = 0$

$$\frac{Z^{\times}(n)}{Z} = \frac{1}{Z} Tr\left(e^{-\beta \mathcal{H}_{BCSOS}} \delta(\delta h = 0)\right) = e^{-\beta f^{\times}(n)}$$

Beijeren isomorphism with the six-vertex m



e^{-K} e^{-K} e^{-K} e^{-K} 1 1

K= β J

- isotropic case - F model (Lieb 1967)
  Kosterlitz-Thouless roughening transition of infinite order at
  $T_R = e^{-K}/(k_B \ln 2) \quad f_{sing} = \exp(-\alpha|T - T_R|^{-1/2})$

XXZ quantum chain

- lines of arrows are labeled by eigenvalues of $2S_j^z$ for spin -1/2

- XXZ Heisenberg - Ising Hamiltonian commutes with the transfer matrix of the F model in $(1,1)$ direction for $\Delta = 1 - (1/2)e^K$ (McCoy and Wu 1968)

$$\mathcal{H}_{XXZ} = J \sum_{j=1}^{M} \left[(S_j^x S_{j+1}^x + S_j^y S_{j+1}^y) + \Delta S_j^z S_{j+1}^z \right]$$

ground state of $\mathcal{H} \rightarrow$ maximum eigenvalue of TM

Emptiness formation probability

Proceeding in the $(1,1)$ direction, the height difference at a separation $r = 2na_0$ for integer n is

$$\delta h = 2\sum_{j=1}^{2n} S_j^z \rightarrow \delta h = 0$$

$$\frac{Z^{\times}(n)}{Z} = \frac{1}{Z} Tr\left(e^{-\beta\mathcal{H}_{XXZ}}\delta(\delta h = 0)\right) = \int_0^{\pi} \frac{d\theta}{\pi} f(\theta, 2n) = e^{-\beta f^{\times}(n)}$$

$$f(\theta, 2n) = \langle \exp\left(i\theta \sum_{j=1}^{2n} S_j^z\right)\rangle_{\mathcal{H}_{XXZ}}.$$

Bosonization analysis

- at large distances

$$\mathcal{H} = \frac{1}{16\pi} \int dx \left[v(\partial_x \Phi)^2 + \frac{1}{v}(\partial_t \Phi)^2 \right].$$

$\Phi(x) \equiv \Phi(x) + 8\pi\alpha$, from Bethe ansatz results for thermodynamics of the chain:

$$\alpha = (\arccos(-\Delta)/4\pi)^{(1/2)} \qquad v = (J a_0 \sin(4\pi\alpha^2))/(2(1-4\alpha^2))$$

$$\begin{aligned} S_j^z &\sim \frac{a_0}{8\pi\alpha} \partial_x \Phi(x) \\ &- A(-1)^j a_0^{1/8\alpha^2} \sin\left(\frac{\Phi(x)}{4\alpha}\right) + \ldots, \end{aligned}$$

$x = j a_0$ and A is a known constant

Bosonization analysis

$$\left\langle e^{i\theta \sum_{j=1}^{n} S_j^z} \right\rangle_{\mathcal{H}} \sim A(\theta)\ (nc)^{(\theta/4\pi\alpha)^2},$$

where $c^{-1}a_0$ is a short-distance cutoff;

$$\begin{aligned} f(\theta, n) &\sim \frac{A(\theta)}{2}(nc)^{-(\theta/4\pi\alpha)^2} \\ &+ (-1)^n \frac{A(\theta - 2\pi)}{2}(nc)^{-((\theta-2\pi)/4\pi\alpha)^2} \end{aligned}$$

for large n:

$$e^{-\beta f^{\times}(n)} \sim \frac{\mathcal{A}}{\sqrt{\log(nc')}}$$

$$\mathcal{F}(r) \sim -\frac{kT}{2r\log(rc'/a_0)}$$

Summary and conclusions

- $d = 2$ allows the interface to have a diffusive structure at the molecular level, ultimate test for the fluctuation effects $\rightarrow 1/r$
- $d = 3$ BCSOS model of a random surface; interface is locally sharp $\rightarrow 1/(r \ln(r/a_0))$
- agreement with the results from the continuum (Gaussian) model of the interface in contact with two **extended** objects *Lehle, Oettel and Dietrich, Europhys. Lett.* **75**, 174 (2006)