

Thermal fluctuations of an interface near a contact line

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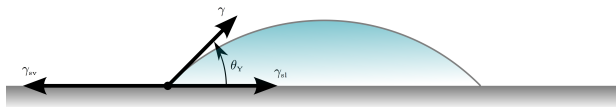
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Introduction

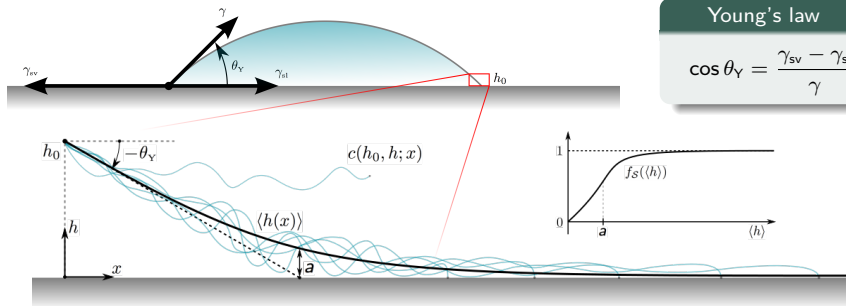
- The understanding and modelling of the dynamics of **wetting and contact lines**, such as spreading or motion of a droplet on a solid surface, is a subject at the forefront of physics, chemistry, and engineering;
- The **regularization** at the contact line is an essential ingredient: within all the descriptions provided in the literature, the physics near the contact line is **oversimplified** since **thermal fluctuations are ignored**;
- Our goal is to **start a different line of thought** to investigate **fluctuating contact lines** at the microscopic scale:
 - 1) **How thermal fluctuations behave** close to a contact line?
 - 2) **Thermal fluctuations alone** can provide any form of **microscopic regularization** within a purely local fluctuating hydrodynamic framework?
- The first step is then to consider a **static contact line** on a homogeneous substrate in presence of **thermal fluctuations**.



Young's law

$$\cos \theta_Y = \frac{\gamma_{sv} - \gamma_{sl}}{\gamma}$$

Mathematical framework



Young's law

$$\cos \theta_Y = \frac{\gamma_{sv} - \gamma_{sl}}{\gamma}$$

Profile probability

$$P_R[h] \propto e^{-\theta_Y^2 \frac{R}{2\ell}} e^{-\frac{1}{2\ell} \int_0^R dx h'(x)^2}$$

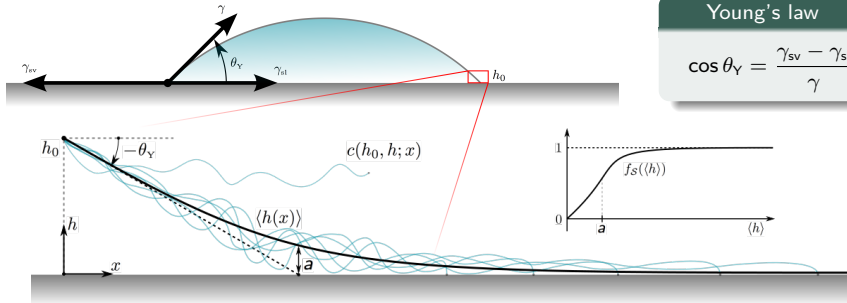
Thermal length

$$\ell = k_B T / \gamma$$

Impenetrability

$$\ell (\partial \ln c / \partial h)_{h=0} = -\theta$$

Mathematical framework



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- Study the statistics of the contact point, i.e. $P(R)$;
- Study the average profiles, i.e. $\langle h(x) \rangle$;
- Quantify the thermal regularization, i.e. a .

Two dimensionless parameters

- $S = \theta_Y h_0 / \ell$ (scale separation): tells us how much thermal fluctuations can distort the interface;
- $\tau = \theta / \theta_Y$ (intensity of interactions): it parametrizes the microscopic binding effects close to the solid substrate.

Thermal length

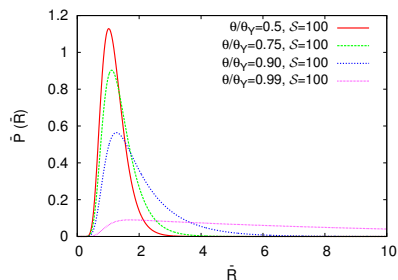
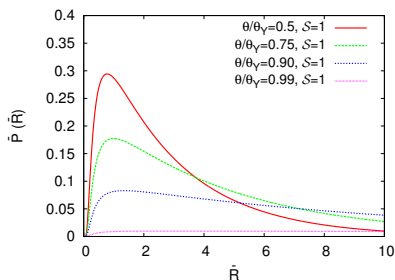
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Impenetrability

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Contact point probability

$$P(R) = \frac{1-\tau}{2} \left[\sqrt{\frac{2S}{\pi R}} e^{S(1-\frac{R}{2}-\frac{1}{2R})} + \tau S e^{S(1-\tau)[1-(1+\tau)\frac{R}{2}]} \operatorname{erfc} \left(\frac{1-\tau R}{\sqrt{2R/S}} \right) \right]$$



Average contact point

$$\langle R \rangle = 1 + \frac{1}{S} \frac{1}{1-\tau}$$

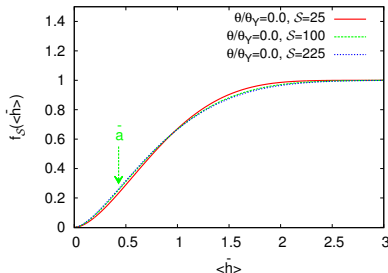
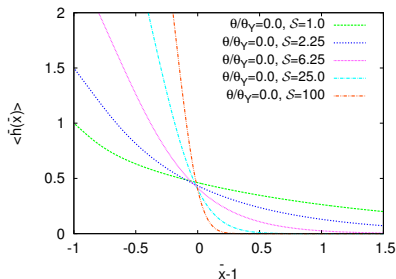
Variance

$$\delta R^2 = \frac{1}{S} \left[1 + \frac{2-\tau}{S(1-\tau)^2} \right]$$

Average profile and binding potential

Average profile

$$\langle h(x) \rangle = \frac{\tau}{(1+\tau)^2} \frac{e^{S(1-\tau)[1-(1+\tau)\frac{x}{2}]} }{\sqrt{S}} \operatorname{erfc}\left(\frac{1-\tau x}{\sqrt{2x/S}}\right) - \frac{x-1}{2/\sqrt{S}} \operatorname{erfc}\left(\frac{x-1}{\sqrt{2x/S}}\right) \\ - \left[\frac{\tau}{(1+\tau)^2} \frac{1}{\sqrt{S}} + \frac{1-\tau}{1+\tau} \frac{x+1}{2/\sqrt{S}} \right] e^{2S} \operatorname{erfc}\left(\frac{x+1}{\sqrt{2x/S}}\right) + \frac{2}{1+\tau} \sqrt{\frac{x}{2\pi}} e^{-\frac{(x-1)^2}{2x/S}}$$



Large x behavior

$$\langle h(x) \rangle \stackrel{x \rightarrow \infty}{\sim} \frac{1}{\sqrt{S}} \frac{2\tau}{(1+\tau)^2} e^{S(1-\tau)} e^{-S(1-\tau^2)\frac{x}{2}}$$

Regularization lengthscale

$$a \stackrel{S \rightarrow \infty}{\sim} \frac{1}{\sqrt{2\pi}}$$

Conclusions

- We have investigated the **effect of thermal fluctuations** on the morphology of an interface **near a contact line** in the presence of an impenetrable wall;
- We have introduced the **right ensemble** (integration over R) where **Young's angle is robust**, and the **inner physics** depends on a boundary condition parameter θ that represents the microscopic deviation from Young's angle;
- The impenetrable nature of the boundary leads to a “repulsion” of capillary waves from the wall and the interactions between the fluctuating interface and the wall are captured in terms of an **effective binding potential** of finite range, **solely induced by thermal fluctuations**;
- **Pseudo-partial wetting states** emerge similarly to a phase transition in the model ($\langle R \rangle \rightarrow \infty$), depending on the micromechanics parameter θ ;
- **Open issue**: Derivation of θ from inner model. Then, and then only, we may expect to predict the conditions under which a pseudo-partial wetting transition can be observed in a real three-dimensional case.

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Thanks for your attention!