Effective contact angle for rough boundary

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ABSTRACT

We provide rigorous justification for the classical Wenzel equation for the roughness enhanced effective contact angle. The minimization of the total surface energy is reformulated into a variational problem. As the size of the roughness becomes small, we show convergence of the minimizer. The limiting minimizer and effective contact angle are explicitly calculated to verify the Wenzel equation.

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1. Introduction

The study of wetting phenomenon on rough surfaces is of critical importance for many industrial applications and has attracted much interest in physics and applied mathematics communities in the past decade. The primary parameter that characterizes wetting is the static contact angle, which is defined as the measurable angle that a liquid makes with a solid. The contact angle of liquid with a flat, homogeneous surface is given by Young’s equation

\[ \cos \theta = \frac{\gamma_{SV} - \gamma_{SL}}{\gamma}, \]  

(1.1)

where \( \gamma_{SV} \), \( \gamma_{SL} \) and \( \gamma \) are the surface tension of the solid–vapor interface, the solid–liquid interface and the liquid–vapor interface respectively. If the liquid wets the surface (referred to as wetting liquid or hydrophilic surface), the value of the static contact angle is \( 0 \leq \theta \leq 90^\circ \), whereas if the liquid does not wet the surface (referred to as nonwetting liquid or hydrophobic surface), the value of the contact angle is \( 90^\circ \leq \theta \leq 180^\circ \). Surfaces with a contact angle between \( 150^\circ \) and \( 180^\circ \) are called superhydrophobic.

For rough surfaces, such as the surfaces with periodic structures shown in Fig. 1, Wenzel [1] proposed an equation for the effective contact angle \( \theta_e \) in terms of static contact angle \( \theta_i \) when the liquid drop is everywhere in contact with the surface. Here \( r \) is the roughness factor (ratio of the actual area to the projected area of the surface). It is shown that \( r \) should be the local roughness factor \( r \) around the contact line [2]. On the other hand, if penetration does not occur and the drop remains balanced on the surface projections with air beneath it, it is in the suspended or Cassie–Baxter state with contact angle

\[ \cos \theta_e = \phi \cos \theta_i - (1 - \phi), \]

with \( \phi \) the solid fraction of the surface. For the smooth but chemically heterogeneous surface, Cassie [3] derived the equation for effective contact angle

\[ \cos \theta_e = \lambda \cos \theta_{i1} + (1 - \lambda) \cos \theta_{i2} \]

in terms of the static contact angles \( \theta_{i1}, \theta_{i2} \) and area fractions \( \lambda \) and \( 1 - \lambda \) of the component surfaces.

There have been many works on the derivation and validity of the Wenzel and Cassie equations [4–12]. Most of the derivations of the Wenzel and Cassie equations are based on the minimization of the total surface energy. In [4], the effective total surface energy is derived from a homogenization argument and bounds for the effective angles can then be derived for various configurations. In [2], the Wenzel and Cassie equations are derived from a phase field model by first deriving an effective boundary condition on the rough surfaces.

There are still many controversies on the two equations [5–9]. The complexity of the problem also comes from the contact angle hysteresis (CAH). The effective contact angle of liquid drops on rough or inhomogeneous surfaces could take a range of values,
where phase $i$ and phase $j$ are the phases in a container occupying a region $\Omega$. Among those possible effective angles, the largest one is called the advancing angle and the smallest is called the receding angle, and the difference between the advancing and receding angle is called contact angle hysteresis. There have been intensive studies on CAH, see [13–16,11] among others, although the theory on CAH is still very much incomplete.

In this paper, we consider the energy minimization problem in a more specific setting so that the limiting minimizer and effective contact angle can be explicitly calculated. We consider only the Wenzel state, i.e., the liquid occupies the spaces between the contact angle can be explicitly calculated. We consider only the Wenzel state, i.e., the liquid occupies the spaces between the surface projections and is everywhere in contact with the surface. We show that when the scale of the roughness approaches zero, energy minimizers have a limit with an effective contact angle modified by the roughness factor of the surface.

The paper is organized as follows. In Section 2, we consider a simple case where the surface is rough in one direction and set up the variational formulation for the energy minimization. We then prove the convergence of the quasi-minimizers in Section 3. Finally, we show the results for rough surfaces with general periodic structures in Section 5.

2. The surface energy and variational formulation

2.1. Surface energy

For a liquid (L)–vapor (V) two phase system in contact with the solid (S) surface, the total interfacial energy can often be written as

$$\sum \sigma_{ij} |\Gamma_{ij}|,$$

where $\sigma_{ij}$ is the surface tension between phase $i$ and phase $j$ and $|\Gamma_{ij}|$ is the area of the surface $\Gamma_{ij}$ which is the interface between the phase $i$ and phase $j$ regions. Consider, for example, two fluids filled in a container occupying a region $\Omega$.

Assume that the container is made of two different materials, $a$ and $b$, so $\partial \Omega$ is decomposed into two parts, $\Pi_a$ and $\Pi_b$ satisfying $\partial \Omega = \Pi_a \cup \Pi_b$, $|\Pi_a \cap \Pi_b| = 0$. Denote by $D \subset \Omega$ the region occupied by the first fluid and by $D' := \Omega \setminus D$ the region occupied by the second fluid. Then the total interfacial energy can be written as

$$\sigma_{12}|\Omega \cap \partial D| + \sigma_{1b}|\Pi_a \cap \partial D| + \sigma_{2a}|\Pi_a \cap \partial D'| + \sigma_{2b}|\Pi_b \cap \partial D'|.$$

Since $|\Pi_a \cap \partial D| + |\Pi_a \cap \partial D'| = |\Pi_a|$, $|\Pi_b \cap \partial D| + |\Pi_b \cap \partial D'| = |\Pi_b|$, the energy can be expressed as

$$\sigma_{12}|\Omega \cap \partial D| + (\sigma_{1a} - \sigma_{2a})|\Pi_a \cap \partial D| + (\sigma_{1b} - \sigma_{2b})|\Pi_b \cap \partial D| + \mathcal{C}$$

where $\mathcal{C} = \sigma_{2a}|\Pi_a| + \sigma_{2b}|\Pi_b|$ is a constant.

Suppose the first fluid is a liquid and the second fluid is the air. Then $\Gamma := \Omega \cap \partial D$ is the air–liquid interface and $\gamma := \sigma_{12}$ is the air–liquid surface tension. Suppose the container is a solid box with an open top (see Fig. 2). We can set $\Pi_a$ as the solid boundary and $\Pi_b$ as the open top, regarded as made of air, so that we can assume without loss of generality that $\Pi_b \cap \partial D = \emptyset$. We call $S := \Pi_a \cap \partial D = \partial \Omega \cap \partial D$ the wet part of solid boundary. Thus, denoting $\sigma_1 = \sigma_{1a}$ the liquid–solid surface tension and $\sigma_2 = \sigma_{2a}$ the air–solid surface tension, up to an additive constant, the total interfacial energy can be written as

$$\sigma |\Gamma| + (\sigma_1 - \sigma_2)|S|$$

where $\Gamma = \Omega \cap \partial D$, $S = \partial \Omega \cap \partial D$.

Assume further that $|\sigma_1 - \sigma_2| < \sigma$, so that there exists a unique $\gamma \in (0, \pi)$ such that $\sigma_2 - \sigma_1 = \sigma \cos \gamma$.

Then the energy can be expressed as

$$\mathcal{E}(D) = \sigma(|\Gamma| - |S| \cos \gamma). \quad (2.1)$$

Note that if $\gamma \in (0, \pi/2)$, then increasing $|S|$ decreases the energy. In this case the solid boundary is called hydrophilic. Similarly, if $\gamma \in (\pi/2, \pi)$, then decreasing $|S|$ decreases the energy, so the boundary is called hydrophobic. The angle $\gamma$ is called the (solid–liquid) contact angle since one can formally derive that for energy minimizers in certain setting, $\gamma$ is the intersection angle of the air–liquid interface $\Gamma = \Omega \cap \partial D$ with the wet part of the solid boundary $S := \partial \Omega \cap \partial D$.

Here we would like to consider the effective contact angle in the case when $\partial \Omega$ is very rough in a microscopic scale.

2.2. A variational formulation

We now set up a variational problem based on a magnification of a local configuration near intersections of air–liquid–solid phases. The microscopic structure of the rough boundary will be taken with a simple form here. More complicated forms will be considered in the subsequent sections.

We consider a liquid drop in the air with one side attached to a solid surface. Pick an arbitrary point of liquid–solid–air intersection. After magnification and rotation near this point we pick a slab of the form $Q := [-1, 1] \times \mathbb{R}^2$. For simplicity, assume...
that the solid boundary in this slab has the form \( x = h(y) \), where \( \varepsilon \) is a small positive constant and \( h \) is a smooth periodic function normalized with its maximum being exactly zero:

\[
\begin{align*}
\max_{y \in [0, 1]} h(y) &= 0. \\
Sonic h may not be smooth (as in Fig. 1), but we assume that it can be approximated by a smooth function. We also assume that there is a function \( u \) such that the air–liquid interface is the surface \( z = u(x, y) \), the fluid in the slab is below the interface, and the air is above the interface (see Fig. 3). Assume for simplicity that \( u \) is \( \gamma \)-periodic with period \( N \varepsilon \) for some positive integer \( N \) and also \( |u| < M \). Then we need only to consider the energy in the tube

\[
[-1, 1] \times [0, N \varepsilon) \times [-M, M].
\]

Scaling the air–liquid surface tension \( \sigma \) by \( 1/(N \varepsilon) \), the interfacial energy of the air–fluid interface can be expressed as

\[
\frac{1}{N \varepsilon} \int_0^{N \varepsilon} \int_{h(y)}^1 \sqrt{1 + |\nabla u|^2} \, dx \, dy.
\]

Scaling the surface tension \( \sigma_2 - \sigma_1 \) by \( \cos \gamma/(N \varepsilon) \), the combined air–solid and liquid–solid interfacial energies in this tube can be combined as

\[
-\frac{\cos \gamma}{N \varepsilon} \int_0^{N \varepsilon} \int_{-M}^M \sqrt{1 + |h_y|^2} \, dy \, dz + C
\]

\[
= -\frac{\cos \gamma}{N \varepsilon} \int_0^{N \varepsilon} \sqrt{1 + |\nabla h(y)|^2} u(h(y), y) \, dy + C_M,
\]

where \( C \) and \( C_M \) are constants. Note that the other surfaces: \( \{ y = 0 \} \), \( \{ y = N \varepsilon \} \), and \( \{ x = 1 \} \), \( \{ x = -M \} \), \( \{ z = M \} \) do not contribute to the interfacial energy that depends on the interface. Thus, the local energy relevant to the air–liquid interface can be written as

\[
\mathbf{E}_0(u) = \frac{1}{N \varepsilon} \int_0^{N \varepsilon} \int_{h(y)}^1 \sqrt{1 + |\nabla u(x, y)|^2} \, dx \, dy
\]

\[
-\frac{\cos \gamma}{N \varepsilon} \int_0^{N \varepsilon} \sqrt{1 + |h_y|^2} u(h(y), y) \, dy.
\]

For simplicity, we assume that the intersection of the air–liquid interface at \( x = 1 \) is flat. By a vertical shifting, we can assume without loss of generality that \( u(1, y) = 0 \). Hence, we consider the energy \( \mathbf{E}_N \) in the function space

\[
\mathbf{X}_{c, N} := \{ u \in W^{1,1}(B_{r, N}) \mid u(x, 0) = u(0, 0), u(1, y) = 0 \}
\]

where

\[
B_{r, N} := \{ (x, y) \mid 0 < y < N \varepsilon, h(y) < x < 1 \}.
\]

Thus, a magnification of a stable configuration near the solid–liquid–air intersection point can be regarded as minimizers of the functional \( \mathbf{E}_N \) in \( \mathbf{X}_{c, N} \). This is the main problem we study in the paper,

\[
\min_{u \in \mathbf{X}_{c, N}} \mathbf{E}_N(u).
\]

2.3. The contact angle

For \( u \in \mathbf{X}_{c, N} \), we extend \( u \) in the \( y \)-direction periodically with period \( N \varepsilon \), and denote by \( \Gamma \) the corresponding air–liquid interface and by \( S \) the wet (solid–liquid) boundary:

\[
\Gamma := \{ (x, y, u(x, y)) \mid y \in \mathbb{R}, h(y) < x < 1 \},
\]

\[
S := \{ (x, y, z) \mid y \in \mathbb{R}, x = h(y), z \leq u(x, y) \}.
\]

Also we take the convention of the unit normal of \( \Gamma \) and \( S \) by

\[
n \equiv (-1, h_y', 0), \quad \hat{n} = \frac{(\nabla u, -1)}{\sqrt{1 + |\nabla u|^2}}.
\]

One can derive that when \( h \equiv 0 \), i.e., the solid surface is flat, the minimizer is given by

\[
u(x, y) = \frac{(1 - x) \cot \gamma = (x - 1) \tan \left( \frac{\gamma}{2} \right).}
\]

This implies that \( \hat{n} \cdot \hat{n} = \cos \gamma \), so \( \gamma \) is intersection angle of the air–liquid interface with the wet part of the solid boundary.

Suppose \( h \) is not a constant function and \{ \( u', \) \} is a family of minimizers. Assume, for simplicity, that for some \( \gamma \in (0, \pi), \)

\[
\lim_{\varepsilon \to 0} u'(x, y) = (1 - x) \cot \gamma = (x - 1) \tan \left( \frac{\gamma}{2} \right).
\]

Since macroscopically the solid boundary \( x = h(y) \) is viewed as \( x = 0 \) and the air–liquid interface \( z = u'(x, y) \) is observed as \( z = (x - 1) \tan(\gamma - \pi/2) \), we observe macroscopically a contact angle \( \hat{\gamma} \). Then, the macroscopically rough surface provides a macroscopically contact angle equal to \( \hat{\gamma} \).

2.4. The reduction to \( N = 1 \)

Here we show that to study energy minimizers of \( \mathbf{E}_N \) in \( \mathbf{X}_{c, N} \), it suffices to consider \( \mathbf{E}_1 \) in \( \mathbf{X}_{c, 1} \).

Theorem 1. The minimization problem of \( \mathbf{E}_N \) in \( \mathbf{X}_{c, N} \) is equivalent to that of \( \mathbf{E}_1 \) in \( \mathbf{X}_{c, 1} \); more precisely, the following holds:

(1) For every \( u \in \mathbf{X}_{c, 1} \), extend \( u \) in the \( y \) direction periodically with period \( \varepsilon \) we have

\[
\mathbf{E}_N[u] = \mathbf{E}_1[u].
\]

(2) For every \( u \in \mathbf{X}_{c, N} \), there exists \( v \in \mathbf{X}_{c, 1} \) such that

\[
\mathbf{E}_1[v] \leq \mathbf{E}_N[u]
\]

where equality holds if and only if \( u \) is a \( \gamma \)-periodic extension of \( v \) with period \( \varepsilon \).
Hence, we have 

\[ E[v, t] = \lim_{t \to 0} \frac{\|v \|_{L^\infty}^p}{t} \]

Since \( E[v, t] \) is a minimizer of \( E^{r,N} \) in \( X_{r,N} \). This completes the proof.  

2.5. The PDE formulation

Suppose \( u \) and \( \zeta \) are smooth functions in \( X_{r,N} \). Then we can calculate the first variation

\[
\frac{\delta E^{r,N}[u]}{\delta u}(\zeta) = \lim_{t \to 0} \frac{E^{r,N}[u + t \zeta] - E^{r,N}[u]}{t}
\]

\[
= \frac{1}{N} \int_0^{Nt} \nabla u \cdot \nabla \zeta \, dx dy
\]

\[
- \cos \gamma \int_0^{Nt} \sqrt{1 + h(y)^2} \, \zeta(h(y), y) dy
\]

\[
= \frac{1}{N} \int_0^{Nt} \left( \frac{u_y}{\sqrt{1 + |\nabla u|^2}} \right) \zeta(\gamma) \, dx.
\]

Thus, if \( u \in X_{r,N} \) is a minimizer of \( E^{r,N} \) in \( X_{r,N} \) and is smooth, then it is a solution of the following boundary value problem:

\[
\begin{align*}
\text{div} \left( \frac{\nabla u}{\sqrt{1 + |\nabla u|^2}} \right) &= 0 & \text{in } B_{r,N}, \\
u(\cdot, 0) &= u(\cdot, N\epsilon), & \text{on } [h_0(\cdot), 1] \times [0, N\epsilon), & (2.7)
v(\cdot, 1) &= 0, & \text{on } [1] \times [0, N\epsilon),
\end{align*}
\]

\[
\begin{align*}
\mathbf{n}_r \cdot \mathbf{n}_S &= \cos \gamma & \text{on } \{h(\cdot, y) \cdot y \in [0, N\epsilon] \}
\end{align*}
\]

If \( u \) is a classical, i.e., \( u \in C^2(B_{r,N}) \cap C^1(\partial B_{r,N}) \), solution of (2.7), then extend \( u \) to \( B_{r,\infty} \) by \( u(x, y + iN\epsilon) = u(x, y) \) for all natural integer \( i \) in the second and third equation in (2.7) implies that \( u \) satisfies the first equation in (2.7) in \( B_{r,\infty} \), so \( u \) is smooth in \( B_{r,\infty} \). In addition, comparing \( u(\cdot, \cdot) \) with \( u(\cdot, \cdot + \epsilon) \), by the strong maximum principle one derives \( u(\cdot, \cdot) = u(\cdot, \cdot + \epsilon) \). Hence, \( u \) is also the unique classical solution of

\[
\begin{align*}
\text{div} \left( \frac{\nabla u}{\sqrt{1 + |\nabla u|^2}} \right) &= 0 & \text{in } B_{r,\infty}, \\
u(\cdot, 0) &= u(\cdot, \cdot + \epsilon), & \text{on } [1] \times \mathbb{R}, & (2.8)
v(\cdot, 1) &= 0, & \text{on } \{x, h(\cdot, y) \cdot y \in \mathbb{R} \}
\end{align*}
\]

Hence, we know the following:

(1) \( \Gamma_r \) is a minimal surface;

(2) \( \Gamma_r \) intersects \( S_r \) at an angle equal to \( \gamma \); i.e., \( \mathbf{n}_r \cdot \mathbf{n}_S = \cos \gamma \) at \( S_r \cap \Gamma_r \).

In general, (2.8) may not admit a solution since the associated minimal surface may not be a z-graph.

3. The Wenzel effective contact angle

In this section we consider the asymptotic limit, as \( \epsilon \to 0 \), of the minimizers of the interfacial energy function

\[
E[v, t] = \int_0^t \int_{h_0(y)}^{h_0(y)} \sqrt{1 + |\nabla u(x, y)|^2} \, dx \, dy
\]

\[- \cos \gamma \int_0^t \sqrt{1 + h(y)^2} \, u(h(y), y) \, dy \]

(3.1)
where for any interval \((a, b)\),
\[
\int_a^b \frac{1}{|b - a|} \int_a^b f(x) \, dx.
\]

Denoting by \(C^{0,1}\) the space of Lipschitz continuous functions, we consider \(E^\epsilon\) in the space
\[
X_\epsilon := \{ u \in C^{0,1}(\bar{B}_\epsilon) \mid u(\cdot, 0) = u(\cdot, \epsilon) \},
\]
\(B_\epsilon := \{(x, y) \mid y \in (0, \epsilon), x \in (h_\epsilon(y), 1)\} \).

Since minimizers of \(E^\epsilon\) are known as only functions of bounded variation (BV), to avoid sophisticated theory of geometry measure, we use quasi-minimizers; that is, those functions \(u' \in X_\epsilon\) that satisfy \(E^\epsilon[u'] < \epsilon + C\), where \(C := \inf_{u \in X} E[u]\). We remark that the regularity of the minimizers is an interesting question. In particular, when \(\epsilon\) is small, the minimizer might be a classic solutions of (2.7). However, this is not the objective of the current paper and will be studied separately.

Also we shall consider the minimization problem under the following condition:
\[
\nu := |\cos \gamma| \max_{y \in [0, 1]} \sqrt{1 + h''(y)^2} < 1. \tag{3.2}
\]

As explained in the next section, if this condition is not satisfied, \(E^\epsilon\) might not have a lower bound. The meaning of the condition is shown in Fig. 4. The contact angle \(\gamma\) should be bigger than \(\theta\) (with \(\tan \theta = h'(y)\) in Fig. 4) and be smaller than \(\pi - \theta\). Otherwise, there might be air trapped below the interface and it will be in the Cassie–Baxter state.

In the following, we will prove some key properties of the energy functional \(E^\epsilon[u]\), including the lower bound and the upper bound of the energy infimum, the estimations of the liquid-interface surface energy integral and the solid surface energy integral, and some other related properties. Finally, we conclude with our main result of this section.

### 3.1. Energy lower bound

Under (3.2), the boundary integral can be estimated by
\[
\lim_{\epsilon \to 0} \int_0^\epsilon \left[ |\cos \gamma| \int_0^1 \sqrt{1 + h''(y)^2} u(h_\epsilon(y), y) \, dy \right] \, dx 
\leq 
\nu \int_0^\epsilon \left[ |u(h_\epsilon(y), y)| \, dy = \nu \int_0^\epsilon \int_{h_\epsilon(y)}^{h_\epsilon(0)} u(x, y) \, dx \, dy \right] \, dy
\]
where in the equation we have used the boundary condition \(u(1, y) = 0\). Thus, we have
\[
E^\epsilon[u] \geq (1 - \nu) \int_0^\epsilon \int_{h_\epsilon(y)}^{h_\epsilon(0)} \sqrt{1 + |\nabla u|^2} \, dx \, dy \quad \forall u \in X_\epsilon. \tag{3.3}
\]

### 3.2. The reduced energy and upper bound of energy infimum

If \(u(x, y) = v(x)\) is a function of one variable, where \(v(x) = v(0)\) for all \(x \leq 0\), we find that
\[
E^\epsilon[v] = \mathcal{E}[v] - \epsilon \tilde{h}, \quad \tilde{h} := \int_0^1 h(Y) \, dY, \tag{3.4}
\]
\[
\left( v(x) := v(0) \text{ when } x < 0 \right)
\]
where \(\mathcal{E}\) is the reduced energy function defined by
\[
\mathcal{E}[v] := \int_0^1 \sqrt{1 + v^2(x)} \, dx - v(0) \cos \gamma, \quad \gamma := \arccos \left( \frac{\int_0^1 \sqrt{1 + h''(y)^2} \, dy}{\sqrt{\int_0^1 (1 + h''(y)^2) \, dy}} \cos \gamma \right). \tag{3.5}
\]

In view of condition (3.2), we see that \(\gamma \in (0, \pi)\) is well-defined. Associated with \(X_\epsilon\), we consider \(E\) in the function space
\[
X := \{ v \in C^{0,1}(\{0, 1\}) \mid v(1) = 0 \}.
\]

The integral in the definition of \(\mathcal{E}\) is the length of the curve \(\{ (x, v(x)) \mid x \in [0, 1] \}\). For any function \(v \in X\), setting \(k = v(0)\) and \(\tilde{u}(x) = k(1 - x)\), we have \(\mathcal{E}[v] \geq \mathcal{E}[\tilde{u}] = \sqrt{1 + k^2} - k \cos \gamma\), where the equals sign holds iff \(v = \tilde{u}\). The minimum of the last quantity is attained at \(k = \cot \gamma\). Hence,
\[
\min_{v \in X} \mathcal{E}[v] = \mathcal{E}[v^\nu] = \sin \gamma, \quad v^\nu(x) = (1 - x) \cot \gamma. \tag{3.6}
\]

Consequently, from (3.4),
\[
\inf_{u \in X} E^\epsilon[u] \leq \min_{v \in X} \mathcal{E}[v] - \epsilon \tilde{h} = \sin \gamma - \epsilon \tilde{h}. \tag{3.7}
\]

This gives the upper bound of the energy infimum.

### 3.3. The average function

For \(u \in X_\epsilon\), we denote by \(\bar{u}\) its average over the \(y\) variable:
\[
\bar{u}(x) = \frac{1}{\epsilon} \int_0^\epsilon u(x, y) \, dy, \quad \forall x \in [0, 1].
\]

The average function plays an important role in the study of the asymptotic limit of functional \(E^\epsilon[u]\).

For every \(y \in [0, \epsilon]\), we can estimate
\[
\int_0^1 |\bar{u}(x) - u(x, y)| \, dx \leq \int_0^1 \int_0^\epsilon |u(x, \bar{y}) - u(x, y)| \, d\bar{y} \, dx
\leq \int_0^\epsilon \int_0^\epsilon |u(y, \bar{y})| \, d\bar{y} \, dx
= \int_0^\epsilon \int_0^\epsilon |u(y, \bar{y})| \, d\bar{y} \, dx.
\]

In view of (3.3), we derive that
\[
\max_{y \in [0, \epsilon]} \|u(\cdot, y)\|_{L^1([0, 1])} \leq \int_0^\epsilon \int_0^1 \sqrt{1 + |\nabla u|^2} \, dx \, dy
\leq \frac{E^\epsilon[u]}{1 - \nu}. \tag{3.7}
\]
3.4. The surface area integral

In this subsection, we will give an estimate of the liquid–vapor interface area integral.

Since \( f(t) = \sqrt{1 + t^2} \) is a convex function, for each \( x \in [0, 1] \), taking
\[
t_0 = \int_0^1 |\nabla u(x, y)| dy > \int_0^1 u(x, y) dy = |\bar{u}_x(x)|,
\]
we obtain for each \( x \in [0, 1] \),
\[
\int_0^1 \sqrt{1 + |\nabla u(x, y)|^2} dy = \int_0^1 f(|\nabla u(x, y)|) dy
\geq \int_0^1 \left( f(t_0) + f'(t_0) |\nabla u(x, y)| - t_0 \right) dy
= f(t_0) \geq \sqrt{1 + |\bar{u}_x(x)|^2}.
\]
Hence, as \( h_x \leq 0 \),
\[
\int_0^1 \int_{h_x(y)}^{1} \sqrt{1 + |\nabla u|^2} \, dx \, dy \geq \int_0^1 \int_0^1 \sqrt{1 + |\nabla u|^2} \, dx \, dy
\geq \int_0^1 \int_0^1 \sqrt{1 + \bar{u}_x(x)^2} \, dx.
\]
(3.8)

3.5. Energy near left boundary

As a preparation for estimating the boundary integral, we establish an estimate near the left end of the boundary (as shown in (3.10)).

For this, let \( u \in \mathbf{X} \), and \( \delta \in (0, 1 \) and define
\[
T_x u(x, y)
= \begin{cases}
0 & \text{when } x \in [1 - \delta, 1], \ y \in [0, \epsilon], \\
u(x + \delta, y) & \text{when } x \in [\delta, y, 1 - \delta], \ y \in [0, \epsilon].
\end{cases}
\]
(3.9)

Comparing the energy of \( u \) and \( T_x u \) we find that
\[
E'[u] - E'[T_x u]
= \int_0^1 \left( \int_{h_x(y)}^{h_x(y) + \delta} \sqrt{1 + |\nabla u|^2} \, dx - \int_{1 - \delta}^{1} \sqrt{1 + |\nabla T_x u|^2} \, dx \right) dy
\geq \int_0^1 \int_{h_x(y)}^{h_x(y) + \delta} \sqrt{1 + |\nabla u|^2} \, dx \, dy
- \cos y \int_0^1 \int_{h_x(y)}^{h_x(y) + \delta} \left( u(h_x(y), y) - u(h_x(y) + \delta, y) \right) dy
\geq (1 - \nu) \int_0^1 \int_{h_x(y)}^{h_x(y) + \delta} \sqrt{1 + |\nabla u|^2} \, dx \, dy
- \delta - \nu \int_0^1 \int_{h_x(y)}^{h_x(y) + \delta} u(x, y) \, dx \, dy
\geq (1 - \nu) \int_0^1 \int_{h_x(y)}^{h_x(y) + \delta} \sqrt{1 + |\nabla u|^2} \, dx \, dy
- \delta - \nu \int_0^1 \int_{h_x(y)}^{h_x(y) + \delta} u(x, y) \, dx \, dy
\geq (1 - \nu) \int_0^1 \int_{h_x(y)}^{h_x(y) + \delta} \sqrt{1 + |\nabla u|^2} \, dx \, dy
- \delta.
\]
Using \( E'[T_x u] \geq C_x \), we then derive the near-boundary estimate
\[
\int_0^1 \int_{h_x(y)}^{h_x(y) + \delta} \sqrt{1 + |\nabla u|^2} \, dx \, dy
\leq \delta + E'[u] - C_x \quad \forall \ u \in \mathbf{X}, \ \delta \in [0, 1].
\]
(3.10)

3.6. The boundary integral

We shall show that in the boundary integral, i.e. the first term of \( E'[u(h_x(y), \ y)] \) can be replace by the constant \( \bar{u}(0) \) without any significant change to the corresponding energy (as shown in (3.15)); here the same as before, \( \bar{u}(x) \) is the average of \( u(x, y) \) over \( y \in [0, \epsilon] \). The following is our estimation.

Firstly, for every \( \eta \in (0, 1) \),
\[
\bar{u}(0) - \int_0^\eta \tilde{u}(x) \, dx = \int_0^\eta \int_0^\eta [u(0, y) - u(x, y)] \, dx \, dy
\leq \int_0^\eta \int_0^\eta |u_x(x, y)| \, dx \, dy
= \int_0^\eta \int_0^\eta \tilde{u}_x(x, y) \, dx \, dy.
\]
(3.11)

Also, for every \( \eta \in [0, \epsilon] \),
\[
\int_0^\eta \tilde{u}(x) \, dx - \int_0^\eta u(x, y) \, dx
= \int_0^\eta \int_0^\eta [u(x, y) - u(x, y)] \, dx \, dy
\leq \int_0^\eta \int_0^\eta \int_0^\eta |u_x(x, y)| \, dx \, dy
= \int_0^\eta \int_0^\eta |u_x(x, y)| \, dx \, dy.
\]
This implies,
\[
\max_{y \in [0, \epsilon]} \int_0^\eta \tilde{u}(x) \, dx - \int_0^\eta u(x, y) \, dx
\leq \int_0^\eta \int_0^\eta |u_x(x, y)| \, dx \, dy.
\]
(3.12)

Finally, we estimate
\[
\int_0^\eta \left| u(h_x(y), y) - \int_0^\eta u(x, y) \, dx \right| \, dy
= \int_0^\eta \left| \int_0^\eta \int_0^\eta [u(h_x(y), y) - u(x, y)] \, dx \, dy \right| \, dy
\leq \int_0^\eta \int_0^\eta \int_0^\eta |u_x(x, y)| \, dx \, dy \, dx
= \int_0^\eta \int_0^\eta |u_x(x, y)| \, dx \, dy.
\]
(3.13)

Combining the above three estimates (3.11)-(3.13), we then conclude that
\[
\int_0^c \left| u(h_x(y), y) - \bar{u}(0) \right| \, dy
\leq \int_0^c \left| u(h_x(y), y) - \int_0^\eta u(x, y) \, dx \right| \, dy
\leq \int_0^c \left| \int_0^\eta u(x, y) \, dx - \tilde{u}(x) \, dx \right| \, dy
\leq \int_0^c \left| \int_0^\eta |u_x(x, y)| \, dx \, dy \right| \, dy
\]
\[
\int_0^c \left| \int_0^\eta |u_x(x, y)| \, dx \, dy \right| \, dy
\leq \max \left\{ 2, \frac{\delta}{\nu} \right\} \int_0^\eta \int_0^\eta \sqrt{1 + |\nabla u|^2} \, dx \, dy.
\]
Taking $\eta = \varepsilon$ and $\delta = \max_{\{c, c_0\}} |\eta - h_c(y)| = \varepsilon[1 + \|h\|_\infty]$ in (3.10) we have $\eta < \delta + h_{\varepsilon}$ and
\[
\int_0^1 |u'(h_{\varepsilon}(y), y) - \bar{u}(0)| \, dy \\
\leq 2 \frac{1}{1 - v} \left( [1 + \|h\|_\infty] \varepsilon + E'[u] - C_{\varepsilon} \right). \tag{3.14}
\]
This then leads to the estimate on the boundary integral that
\[
\left| \cos \gamma \int_0^1 \sqrt{1 + h_{\varepsilon}'(y)^2} u(h_{\varepsilon}(y), y) \, dy - \bar{u}(0) \cos \hat{\gamma} \right| \\
= \left| \cos \gamma \int_0^1 \sqrt{1 + h_{\varepsilon}'(y)^2} (u(h_{\varepsilon}(y), y) - \bar{u}(0)) \, dy \right| \\
\leq \gamma \varepsilon \int_0^1 \left( [1 + \|h\|_\infty] \varepsilon + E'[u] - C_{\varepsilon} \right). \tag{3.15}
\]
Combining this estimate with the surface area integral estimate (3.8), we then conclude that
\[
\varepsilon |\bar{u}| \leq E'[u] + \frac{2}{1 - v} \left( [1 + \|h\|_\infty] \varepsilon + E'[u] - C_{\varepsilon} \right), \tag{3.16}
\]
This characterizes the relation of the energy functional $E'[u]$ and the reduced energy $\varepsilon |\bar{u}|$ at the corresponding average function $\bar{u}$.

3.7. Main result

We can summarize our estimate in above subsections as follows:

**Theorem 2.** Assume that (3.2) and (2.2) hold. Then the following holds:

1. Let $X = \{v \in C^1((0, 1)) \mid v(0) = 0\}$, $E[v] = \int_0^1 \sqrt{1 + v_x^2} \, dx - v(0) \cos \gamma$ with $\hat{\gamma}$ a positive angle, Then
   \[
   \min_{v \in X} \varepsilon[v] = \varepsilon[v^*] = \sin \hat{\gamma}, \quad v^*(x) = (1 - x) \cot \hat{\gamma}.
   \]
2. Let $h = \int_0^1 H(y) \, dy$ and choose a specific $\hat{\gamma} = \arccos \left( \int_0^1 \sqrt{1 + h(Y)^2} \, dy \cos \gamma \right)$. Then we have
   \[
   C_{\varepsilon} := \inf_{u \in X} E'[u] \leq \min \varepsilon[v] - \varepsilon \sin \hat{\gamma} - h.
   \]
3. Denote $\|h\|_\infty = \max_{y \in [0, 1]} |h(y)|$ and assume that $0 < \varepsilon < \varepsilon_0 := 1/\|h\|_\infty$. If $u^* \in X$ is a quasi-minimizer of $E'$ in $X$, in the sense that $E'[u^*] \leq \varepsilon + \inf_{u \in X} E'[u]$, then the function of its $y$-average $u^*(\cdot) := \int_0^1 u^*(\cdot, y) \, dy$ satisfies
   \[
   \varepsilon |u^*(\cdot)| \leq E'[u^*] + \frac{2}{1 - v} \left( [1 + \|h\|_\infty] \varepsilon + E'[u^*] - C_{\varepsilon} \right).
   \]
4. Let $\{u^*\}_{0 < c < c_0}$ be a family of quasi-minimizers as above. Then $\{u^*\}_{0 < c < c_0}$ is a minimizing family of $\varepsilon$ in $X$. Consequently,
   \[
   \lim_{c \to 0, c \in (0, 1]} \varepsilon \sin \gamma - v^*(x) = 0, \\
   \lim_{c \to 0, c \in (0, 1]} \varepsilon \sin \gamma - v^*(x) = 0.
   \]

From assertion (2) we now have the Wenzel equation
\[
\cos \gamma = \int_0^1 \sqrt{1 + h'(Y)^2} \, dv \cos \gamma = r \cos \gamma,
\]
where $\gamma$ is the effective contact angle and $r = \int_0^1 \sqrt{1 + h(Y)^2} \, dv$ gives the surface roughness factor.

**Proof.** It remains to prove the consequence part of assertion (4).

Define $k_{\varepsilon} = \bar{u}^*(0)$ and $v^*(x) = k_{\varepsilon}(1 - x)$. Then $E[\bar{u}^*] > \varepsilon|v^*| = \sqrt{1 + k_{\varepsilon}^2} - k_{\varepsilon} \cos \hat{\gamma}$, which, as a function of $k_{\varepsilon}$, attains its global minimum $\hat{\gamma}$ only at the unique value $\cot \hat{\gamma}$. Hence, we derive from
\[
\lim_{\varepsilon \to 0} \varepsilon \sin \hat{\gamma} = \sin \hat{\gamma} \sin \gamma \quad \sin \hat{\gamma} = \sin \gamma.
\]
Next, let $\bar{u}^*(0)$ be a point at which $\varepsilon |\bar{u}^*(0) - v^*(0)|$ attains its maximum. Then the integral $\int_0^1 \sqrt{1 + |\bar{u}^*(x) - v^*(x)|^2} \, dx$ is no smaller than the sum of the lengths of two line segments from $(0, \bar{u}^*(0))$ to $(x, \bar{u}^*(x))$ and from $(x, \bar{u}^*(x))$ to $(1, 0)$. Comparing this sum with the length of the line segment connecting $(0, \bar{u}^*(0))$ and $(1, 0)$ we then derive from the triangular inequality that
\[
\lim_{\gamma \to 0} \left( \varepsilon |\bar{u}^*(x) - v^*(x)| \right) = \lim_{\gamma \to 0} \left( \varepsilon |\bar{u}^*(x) - v^*(x)| \right) = 0.
\]
Finally from (3.7) we obtain the last assertion of the theorem. \(\square\)

3.8. Necessity of condition (3.2)

Here we illustrate that condition (3.2) is necessary. For this, we assume that $\gamma \in (0, \pi/2)$. Consider a special case when
\[
h(Y) = \begin{cases} 0 & \text{if } |Y| \leq \delta, \\ m(|Y| - \delta) & \text{if } |Y| > \delta,
\end{cases}
\]
where $\delta$ is a small number. We fix $m > 0$ such that $\sqrt{1 + m^2} \cos \gamma > 1$.

Note that
\[
\int_0^1 \sqrt{1 + h'(Y)^2} \, dv = 1 + 2(\sqrt{1 + m^2} - 1) = 1 + O(\delta).
\]
It follows that when $\delta$ is positive and small,
\[
\beta = \arcsin \left( \cos \gamma \int_0^1 \sqrt{1 + h(Y)^2} \, dv \right) = \frac{\pi}{2} - \gamma + O(\delta).
\]

Let $K > 0$ be a constant number and consider the test function $u_k = \min(K x, 0)$.

Then we find that
\[
E'[u_k] = 1 + \sqrt{1 + K^2} m \delta^2 - K \cos \gamma \sqrt{1 + m^2} m \delta^2 K \\
= 1 + m \delta^2 K \left( \frac{\sqrt{1 + K^2}}{K} - \cos \gamma \sqrt{1 + m^2} \right).
\]
We find that
\[
\lim_{K \to \infty} \frac{E'[u_k]}{K} = m \delta^2 \left( 1 - \sqrt{1 + m^2} \cos \gamma \right) < 0.
\]
Hence,
\[
\inf_{u \in X} E'[u] = -\infty.
\]

In physics, when condition (3.2) does not hold, air pockets may form. The effective contact angle should be modified by the so-called Cassie–Baxter equation. We will not discuss this situation in this paper.
4. Rough boundary with general periodic microscopic structure

In this section we consider the effective contact angle for a rough boundary with general periodic microscopic structure. For this we consider a liquid in the domain

\[ \Omega_\varepsilon = \{(x, y, z) \mid z \in \mathbb{R}, y \in \mathbb{R}, h_\varepsilon(y, z) < x < 1\} \]

where \( h_\varepsilon(\cdot, \cdot) \) is a smooth function that is periodic in both variables:

\[ h_\varepsilon(y, z) = \varepsilon h \left( \frac{y}{\varepsilon}, \frac{z}{\varepsilon} \right). \tag{4.1} \]

\( h(Y + 1, Z) = h(Y, Z) = h(Y, Z + L), \max_{[0,1) \times [0,1]} h = 0, \)

where \( L \) is a fixed positive constant. We use notation

\[ H = \max_{y \in [0,1], z \in (0,1)} |h(Y, Z)|, \]

\[ A = \int_0^1 \int_0^1 \sqrt{1 + \nabla h(Y, Z)^2} dZ dY. \tag{4.2} \]

In the sequel, the set \( \{(x, y, z) \in \Omega_\varepsilon \mid \text{equations}\} \) is often simply expressed as \{equations\}.

4.1. The energy

Assume that in \( \Omega_\varepsilon \), the \( \text{(air–liquid)} \) interface is given by \( z = u(x, y) \), the liquid region is given by \( z < u(x, y) \) and the air region is \( z > u(x, y) \), where \( u \) is defined on \([-\varepsilon H, 1] \times \mathbb{R} \) and is periodic in \( y \) with period \( \varepsilon \). The interface in one period region can be expressed as

\[ \Gamma_u := \{(x, y, u(x, y)) \mid (x, y) \in B_u\}, \]

\[ B_u := \{(x, y) \mid 0 < y < \varepsilon, h_\varepsilon(y, u(x, y)) < x < 1\}. \]

Here \( B_u \) is the projection of \( \Gamma_u \) on the \( x-y \) plane. Thus, the interfacial energy of the interface is

\[ \frac{1}{\varepsilon} |\Gamma_u| = \frac{1}{\varepsilon} \iint_{B_u} \sqrt{1 + \nabla u(x, y)^2} dxdy. \]

The solid boundary in one period is

\[ S = \{h_\varepsilon(\cdot, y, z, y, z) \mid 0 < y < \varepsilon, z \in \mathbb{R}\}. \]

The wet (part of the solid) boundary is

\[ S_u := \{h_\varepsilon(y, z, y, z) \mid (y, z) \in \Pi_u\}, \]

\[ \Pi_u := \{(y, z) \mid 0 < y < \varepsilon, z < u(h_\varepsilon(y, z), y)\}. \]

Here \( \Pi_u \) is the projection of \( S_u \) on the \( y-z \) plane (see Fig. 5).

To obtain the bounded energy, we assume that \( \|u\|_{\infty} < M \) for some \( M > 0 \) and consider the configuration in the set \([-M < z < 0]\). Substracting from the energy of solid boundary the constant \( C_M = \frac{\varepsilon}{\varepsilon H} |S \cap \{-M < z < 0\}| \), the adjusted energy from the solid boundary is

\[ -\frac{\cos \gamma}{\varepsilon} |S_u \cap \{z > -M\}| + C_M \]

\[ = -\frac{\cos \gamma}{\varepsilon} \left| (S_u \cap \{z \geq 0\}) - (S \backslash S_u) \cap \{z < 0\} \right|. \]

This is (the difference of) surface tension (of dry surface and wet surface) times the signed area of the wet region that differs from the reference region \( S \cup \{z < 0\} \). Hence, we consider the energy

\[ \mathcal{E}'[u] := \frac{1}{\varepsilon} \iint_{B_u} \sqrt{1 + |\nabla u|^2} dxdy \]

\[ -\frac{\cos \gamma}{\varepsilon} \iint_{\Pi_u^+ \cup \Pi_u^-} \text{sgn}(z) \sqrt{1 + |\nabla h_\varepsilon|^2} dxdy \quad (4.3) \]

where \( \text{sgn}(\cdot) \) is the signature function: \( \text{sgn}(z) = 1 \) for \( z \geq 0 \) and \( \text{sgn}(z) = -1 \) for \( z < 0 \), and

\[ \Pi_{u+} := \{(y, z) \mid 0 < y < \varepsilon, 0 < z < u(h_\varepsilon(y, z), y)\}, \]

\[ \Pi_{u-} := \{(y, z) \mid 0 < y < \varepsilon, u(h_\varepsilon(y, z), y) < z < 0\}, \]

\[ \Pi_{0+} := \{(y, z) \mid 0 < y < \varepsilon, u(h_\varepsilon(y, z), y) = z < 0\}. \]

The energy is to be minimized in the space of Lipschitz continuous \((C^{0,1})\) functions: either

\[ \mathcal{X}_e = \{u \in C^{0,1}([-\varepsilon H, 1] \times [0, \varepsilon]) \mid u(\cdot, 1) = 0, u(0, \cdot) = u(\cdot, \varepsilon)\} \]

or

\[ \mathcal{X}_e = \{u \in C^{0,1}([-\varepsilon H, 1] \times [0, \varepsilon]) \mid u(\cdot, 1) = 0\}. \]

We will consider the following variational problem

\[ \inf \mathcal{E}'[u]. \quad (4.6) \]

We will mainly consider the asymptotic behavior of problem when \( \varepsilon \to 0 \).

4.2. Interface or wet boundary?

The surface \(\{h_\varepsilon(y, z, y, z) \mid (y, z) \in \Pi_{0+}\} \) is a subset of the intersection of the solid boundary \(\{x = h_\varepsilon(y, z, y, z)\}\) and the surface \(\{z = u(x, y)\}\). This set can be regarded as a wet (solid) boundary, dry boundary, and/or (air–fluid) interface. Let \( p \) be a Lebesgue point of the intersection. Consider two situations:

(1) Suppose the interior normal of the solid boundary \( \Pi \) at \( p \) points downwards. Then an infinitesimal lift-up of \( u \) near \( p \) makes the solid surface near \( p \) a well-defined wet boundary, whereas an infinitesimal push-down of \( u \) makes the graph \( z = u \) near \( p \) a well-defined wet boundary.

If \( y \in (0, \pi/2] \), then the infinitesimal lift-up of \( u \) gives energy smaller than that of push-down, so this intersection near \( p \) can be regarded as a wet boundary.

If \( y \in (\pi/2, \pi) \), then neither the infinitesimal lift-up (adding wet boundary but no interface) nor the infinitesimal push-down (adding interface but no wet boundary) decreases the energy, so there is no unique way to interpret this intersection near \( p \) as a wet boundary and/or interface.

(2) Suppose the interior normal of \( \Pi \) points upwards. Then an infinitesimal push-down of \( u \) makes the surface near \( p \) a dry boundary, whereas an infinitesimal lift-up produces one piece of wet boundary and another piece of interface with infinitesimal distance between them. This provides a net
increase in energy from treating it as a dry boundary since the ratio of the energy densities of a wet boundary and interface is \( \cos \gamma \). Thus the default is to treat the intersection near \( p \) as a dry boundary.

Although there are the above complications, the total area of surface in question is negligible as shown below:

**Lemma 4.1.** Let \( S \Gamma \) be the intersection of the solid boundary \( x = h_i(y, z) \) with the surface \( z = u(y, x) \). Then with \( A \) defined as in (4.2),
\[
|S \Gamma| \leq c \int_0^\epsilon \int_0^\epsilon \sqrt{1 + |\nabla f(y, z)|^2}dxdy = A \epsilon^2.
\]

**Proof.** Map every \((y, x, z) \in S \Gamma \) to a point \((x, y, \bar{z}) \in \Pi^1 \), where \( \bar{z} \in [0, Le] \) and \( \bar{z} - z \) is an integer multiple of \( Le \). The map is area preserving and one-to-one since \( S \Gamma \) is a z-graph. Hence, the total surface area of \( S \Gamma \) is no larger than the area of the surface \( \Pi^1 \cap \{0 \leq z \leq Le \} \). The assertion of the lemma thus follows.

### 4.3. Lower bound of energy

The same as before, we assume that \( v := \cos \gamma \max_{\{0,1\} \times \mathbb{R}} \sqrt{1 + |\nabla h|^2} < 1 \). (4.7)

**Lemma 4.2.** Assume that (4.7) holds. Then for every \( u \in \mathbf{X} \), defined either by (4.4) or (4.5),
\[
E'[u] \geq \frac{1}{\epsilon} \int_{B_{\epsilon}} \sqrt{1 + |\nabla u|^2}dxdy - A \epsilon.
\]

Consequently, the infimum of the energy \( E' \) in \( \mathbf{X} \), is finite:
\[
C_\epsilon := \inf_{u \in \mathbf{X}} E'[u] > -\infty.
\]

**Proof.** Denote by \( \mathbf{P} \) the projection on the \( y-z \) plane. Then
\[
\mathbf{P}(\Gamma) = \left\{ (y, z) \mid 0 < y < \epsilon, \exists x \in (h_i(y, z), 1) \text{ s.t. } z = u(x, y) \right\}.
\]

It is a simple geometric fact that \( |\mathbf{P}(\Gamma)| \leq |\Gamma| \). Also, since \( u(\cdot, y) = 0 \), by continuity of \( u(\cdot, y) \), we see that \( \Pi^1_+ \cup \Pi^1_- \subseteq \mathbf{P}(\Gamma) \),
\[
|\Pi^1_+| + |\Pi^1_-| \leq |\mathbf{P}(\Gamma)| \leq |\Gamma|.
\]

Hence, the energy resulting from the solid boundary can be bounded by
\[
\frac{\cos \gamma}{\epsilon} \int_{\Pi^1_+ \cup \Pi^1_- \cup \Pi^0_+} \text{sgn}(z) \sqrt{1 + |\nabla h_i|^2}dxdydz
\leq \frac{\epsilon}{\epsilon} \left( |\Pi^1_+| + |\Pi^1_-| \right) + \frac{\cos \gamma}{\epsilon} |S \Gamma| \leq \frac{\epsilon}{\epsilon} |\Gamma| + A \epsilon.
\]

Thus,
\[
E'[u] \geq \frac{1}{\epsilon} |\Gamma_\epsilon| - \frac{\epsilon}{\epsilon} |\Gamma_\epsilon| + A \epsilon = 1 - \frac{\epsilon}{\epsilon} \int_{B_{\epsilon}} \sqrt{1 + |\nabla u|^2}dxdy - A \epsilon.
\]

The assertion of the lemma thus follows.

### 4.4. Near-boundary energy estimate

The same as before, for \( \delta \in (0, 1) \), we consider the shift function \( T^\delta u \) defined by
\[
T^\delta u(x, y) = \begin{cases} 0 & \text{if } y \in [0, \epsilon], x \in [1 - \delta, 1], \\ u(x + \delta, y) & \text{if } y \in [0, \epsilon], x \in [1 - \delta, 1]. \end{cases}
\]

The surface \( \Gamma_{\epsilon} \cap \{1 - \delta < x \leq 1\} \) is \( (0, \epsilon) \times \{0\} \) of area \( \epsilon \).

The graph \( \Gamma_{\epsilon} \cap \{x < 1 - \delta\} \) is obtained by shifting the graph \( \Gamma \) to the left by \( \delta \). It is identical to the restriction of \( \Gamma \) in the new domain obtained by shifting the left boundary \( x = h_i(y, z) \) of the original domain \( \Omega \), to the right by \( \delta \), hence,
\[
|\Gamma_{\epsilon} \cap \{x < 1 - \delta\}| = \epsilon \delta + |\Gamma_{\epsilon} \cap \{h_i(y, z) + \delta < x < 1\}|
\]

Consequently,
\[
|\Gamma_{\epsilon} \cap \{x < 1 - \delta\}| - \epsilon \delta - |\Gamma_{\epsilon} \cap \{h_i(y, z) + \delta < x < 1\}|
\]

Next, we calculate the symmetric difference of \( S_u \) and \( S_{T^\delta u} \). For this, we find that
\[
\Pi_u \setminus \Pi_{T^\delta u} = \{(y, z) \mid 0 < y < \epsilon, u(h_i(y, z), y) > z \}
\]
\[
\Pi_{T^\delta u} \setminus \Pi_u = \{(y, z) \mid 0 < y < \epsilon, u(h_i(y, z) + \delta, y) > z \}
\]
In view of (4.2) and the definition of \( S \Gamma_u \), we find that
\[
\left( \Pi_u \setminus \Pi_{T^\delta u} \right) \cup \left( \Pi_{T^\delta u} \setminus \Pi_u \right) \subseteq \mathbf{P}(\Gamma_u) \times \mathbf{P}(\Gamma_u \cap \{x < h_i(y, z) + \delta\})
\]
where \( \mathbf{P} \) is the projection onto \( y-z \) plane. Hence,
\[
\frac{\cos \gamma}{\epsilon} \left( |S_u \setminus \mathbf{P}_{T^\delta u} \setminus |S_{T^\delta u} \setminus S_u \right)
\]
\[
\leq \frac{\epsilon}{\epsilon} |\Gamma_u \cap \{x < h_i(y, z) + \delta\}| + A \epsilon.
\]
Consequently,
\[
E'[T^\delta u] - E'[u] \leq \frac{1}{\epsilon} \left( |\Gamma_{\epsilon} \cap \{x < h_i(y, z) + \delta\}| + A \epsilon \right)
\]
Using \( E'[T^\delta u] \geq C_\epsilon := \inf_{u \in \mathbf{X}} E'[u] \), we then obtain the following:

**Lemma 4.3.** For every \( \delta \in (0, 1) \),
\[
|\Gamma_u \cap \{x < h_i(y, z) + \delta\}| \leq \frac{E'[u] - C_\epsilon + \delta + A \epsilon}{1 - \nu} \epsilon.
\]

Consequently, if \( u' \) is a quasi-minimizer in the sense that \( E'[u] \leq C_\epsilon + \epsilon \), setting \( \delta = \epsilon + \epsilon H \) and assuming that \( \epsilon < 1/(1 + H) \), we obtain
\[
\int_0^\epsilon \int_0^\epsilon \sqrt{1 + |\nabla u'|^2}dxdy
\leq (\Gamma_u \cap \{x < h_i(y, z) + \delta\}) \leq A_1 \epsilon^2,
\]
\[
A_1 := \frac{2 + H + A}{1 - \nu}.
\]

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4.5. Small oscillation of quasi-minimizer

Assume that \( u \) is a quasi-minimizer. Then by (4.10) and the mean value theorem there exists \( x_\varepsilon \in [0, \varepsilon] \) such that

\[
\int_0^\varepsilon |u'_\varepsilon(x_\varepsilon, y)| \, dy = \int_0^\varepsilon \int_0^\varepsilon |u'_\varepsilon(x, y)| \, dx \, dy \leq A_\varepsilon \varepsilon. 
\]

Define

\[ m_\varepsilon = \min_{[0, \varepsilon]} u(x_\varepsilon, \cdot), \quad M_\varepsilon = \max_{[0, \varepsilon]} u(x_\varepsilon, \cdot). \]

Then we have

\[ M_\varepsilon - m_\varepsilon \leq \int_0^\varepsilon |u'_\varepsilon(x_\varepsilon, y)| \, dy \leq A_\varepsilon \varepsilon. \tag{4.11} \]

4.6. The reduced energy

Let \( u \) be a quasi-minimizer. Define

\[ \tilde{u}(x) := \int_0^x u(x, y) \, dy \quad \forall x \in [0, 1], \quad \tilde{u}(x) = \tilde{u}(0) \quad \forall x < 0. \]

We want to compare the energy of \( u \) and \( \tilde{u} \).

First of all, there is the interface energy comparison

\[
\frac{1}{\varepsilon} |I_u \cap [0 < x < 1]| = \int_0^1 \int_0^1 \sqrt{1 + |\nabla u|^2} \, dx \, dy \\
\geq \int_0^1 \sqrt{1 + \tilde{u}'_0^2(x)} \, dx. \tag{4.12} \]

Next, we compare the boundary energy of \( u \) and \( \tilde{u} \). Note that

\[
S_\tilde{u} = \{(h, y, z) \mid z < \tilde{u}(0) \} = \{z \mid z < \tilde{u}(0) \}.
\]

Consequently,

\[
S_\tilde{u} \setminus S_u = \{(h, y, z) \mid 0 < y \varepsilon, \tilde{u}(0) \leq z < u(h(x, y), y) \} \subseteq \left(1 \subseteq \{z \mid z < \tilde{u}(0) \} \cup \{(h, y, z) \mid 0 < y \varepsilon, M_\varepsilon < z < u(h(x, y), y) \}
\]

Since \( \max u(x_\varepsilon, \cdot) \leq M_\varepsilon \), if \((y, z)\) satisfies \( M_\varepsilon < z < u(h(x, y), y)\), then there exists \( x \in (h(x, y), x_\varepsilon) \) such that \( z = u(x, y) \).

Hence, projecting onto the \( y-z \) plane we obtain

\[
P(S_\tilde{u} \setminus S_u) \subset (0, \varepsilon) \times \{\tilde{u}(0), M_\varepsilon\} \cup P(I_u \cap \{x < x_\varepsilon\}). \tag{4.13} \]

Here \( \{\tilde{u}(0), M_\varepsilon\} \) is an empty set of \( \tilde{u}(0) > M_\varepsilon \). Similarly, since \( \min u(x_\varepsilon, \cdot) = m_\varepsilon \),

\[
P(S_\tilde{u} \setminus S_u) = \{(y, z) \mid 0 < y \varepsilon, \tilde{u}(0) > z \geq u(h(x, y), y) \} \subset (0, \varepsilon) \\
\times [m_\varepsilon, \tilde{u}(0)] \cup \{(y, z) \mid 0 < y \varepsilon, m_\varepsilon > z \geq u(h(x, y), y) \} \subset (0, \varepsilon) \\
\times [m_\varepsilon, \tilde{u}(0)] \cup \{P(I_u \cap \{x < x_\varepsilon\}) \cup P(S_\tilde{u} \setminus S_u). \tag{4.14} \]

Here \( [m_\varepsilon, \tilde{u}(0)] \) is an empty set if \( M_\varepsilon > \tilde{u}(0) \). Hence,

\[
P(S_\tilde{u} \setminus S_u) \subset (0, \varepsilon) \\
\times [m_\varepsilon, M_\varepsilon] \cup \{P(I_u \cap \{x < x_\varepsilon\}) \cup P(S_\tilde{u} \setminus S_u). \tag{4.15} \]

Using further the assumption (4.7), Lemma 4.1, (4.10) and (4.11), we have

\[
|\cos \gamma \|S_u \Delta S_u\| = \int_{P(S_u \setminus S_\tilde{u})} |\cos \gamma \|1 + |\nabla h|^2| \, dydz \\
\leq \varepsilon |\varepsilon| |P(S_u \setminus S_\tilde{u})| \leq \varepsilon |M_\varepsilon - m_\varepsilon| \\
+ |I_u \cap \{x < x_\varepsilon\}| + A_\varepsilon^2 \leq 3A_1 \varepsilon^2. 
\]

Combining with the equation (4.12), it then follows that

\[
E'[\tilde{u}] - E'[u] \leq \frac{1}{\varepsilon} |\cos \gamma \|S_u \Delta S_u\| \leq 3A_1 \varepsilon. \tag{4.16} \]

Finally, using the periodicity of \( h \) we find that

\[
|\cos \gamma \int_{\mathcal{P}_0 \cup \mathcal{P}_0 \cup \mathcal{P}_0} |\text{sgn}(z) \sqrt{1 + |\nabla h|^2|} \, dydz \\
= \frac{\cos \gamma}{\varepsilon} \int_0^1 \int_0^1 \frac{\tilde{u}(0)}{1 + \sqrt{1 + |\nabla h|^2}} \, \sqrt{1 + \sqrt{1 + |\nabla h|^2}} \, dydz \\
= \left[ \frac{\tilde{u}(0)}{L} + \theta \varepsilon \right] A \cos \gamma, 
\]

where \( \theta \in (-1/2, 1/2) \). Hence, we define the reduced energy functional

\[
\mathcal{E}[v] = \int_1^1 \sqrt{1 + v_\varepsilon^2} \, dx - v(0) \cos \gamma, \tag{4.17} \]

where

\[
\gamma = \arccos \frac{A \cos \gamma}{L} \\
= \arccos \left( \int_0^1 \int_0^1 \sqrt{1 + |\nabla h(Y, Z)|^2} \, dYdZ \cos \gamma \right). \tag{4.18} \]

If \( u \) is a quasi-minimizer, we obtain from our previous derivation that

\[
\mathcal{E}[\tilde{u}] - \mathcal{E}'[u] \leq 4A_1 \varepsilon. \tag{4.19} \]

4.7. Main result

Following the same argument as in the previous section we can now conclude the following:

**Theorem 3.** Assume that (4.1) and (4.7) hold. Then the following holds:

1. The energy \( \mathcal{E} \) defined in (4.17) admits a unique minimizer in \( X = \{v \in C^1([0, 1]) \mid (0, 0) = 0\} \):

\[
\min \mathcal{E}[v] = \mathcal{E} [v^*] \sin \gamma, \quad v^*(x) = (1 - x) \cot \gamma.
\]

2. The infimum of \( \mathcal{E}' \) in \( X \) defined either by (4.4) or by (4.5) satisfies

\[
C_e := \inf_{u \in X} \mathcal{E}'[u] \leq \min \mathcal{E}[v] + He + A_\varepsilon \\
= \sin \gamma + He + A_\varepsilon.
\]

Here \( H \) and \( A_\varepsilon \) are constants given in (4.2).

3. Denote \( A_1 = (2 + H + A_\varepsilon)/(1 - v) \) and assume \( 0 < \varepsilon < \varepsilon_0 := 1/(1 + H) \). If \( u^e \in X \), is a quasi-minimizer of \( \mathcal{E}' \) in \( X \), in the sense that \( \mathcal{E}'[u^e] \leq \varepsilon + C_e \), then its \( y \)-average

\[
\bar{u}^e(y) := \frac{1}{\varepsilon} \int_0^\varepsilon u^e(\cdot, y) \, dy 
\]

satisfies

\[
\mathcal{E}[\bar{u}^e] \leq \mathcal{E}[u^e] + 4A_1 \varepsilon \leq \min \mathcal{E}[v] + 5A_1 \varepsilon.
\]
(4) Let \( \{u^\varepsilon\}_{\varepsilon>0} \) be a family of quasi-minimizer as above. Then \( \{u^\varepsilon\}_{\varepsilon>0} \) is a minimizing family of \( \varepsilon \) in X. Consequently,

\[
\lim_{\varepsilon \to 0} \max_{x \in [0,1]} |u^\varepsilon(x) - v^*(x)| = 0,
\]

\[
\lim_{\varepsilon \to 0} \max_{y \in [0,1]} \|u^\varepsilon(\cdot, y) - v^*(\cdot, y)\|_{L^1(0,1)} = 0.
\]

The contact angle \( \gamma \) (defined in (4.18)) is the Wenzel effective contact angle in the general case.

**Remark 4.1.** It is easy to generalize our results to the cases when the (macroscopic) interface is not parallel to the direction of the solid surface heterogeneity. For example, we consider the heterogeneity is of laminate type, with the lamination in the direction \( (0, 1, c) \) instead of the \( y \) direction. The rough surface is given by \( x = \varepsilon h(x^\varepsilon) \), such that \( h(\cdot) \) is a periodic function with period 1. It is easy to see that \( h(Y, Z) = h(Y + cZ) \) is periodic in \( Y \) and periodic in \( Z \) with period 1 and \( 1/c \) respectively. The function \( h \) satisfies the assumptions in Eq. (4.1). Therefore the results in Theorem 3 are correct for the oblique laminate surface. The conclusion is also true for more general cases.

5. Conclusion

We have provided a rigorious justification of the classical Wenzel equation for the roughness enhanced effective contact angle. By studying a variational problem based on surface energy, we show convergence of the energy minimizer and a reduced problem is then derived which provides the effective contact angle. The procedure can be easily generalized to prove the Cassie equation for chemically patterned surfaces. We remark that for real surfaces, \( h_y \) may be non-periodic or even random. We have not considered such cases in this paper. But we note that our results can be generalized to the case where \( h_y \) is only locally periodic in the fast variable \( Y \) [2]. We also note that the minimizers that give rise to the Wenzel effective contact angle are the global minimizers of the energy functional. For rough surfaces, there are also local minimizers. When the scale of the roughness \( \varepsilon \) is not small, the system may attain these local minimizers which give rise to stick-slip motion and contact angle hysteresis in the moving contact line problem [17,18,16].

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**References**