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Effective and microscopic contact angles in thin film dynamics

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We introduce and analyse a class of quasi-self-similar solutions of the thin film equation to describe the dynamics of expanding liquid films on a solid surface. Using these solutions as intermediate asymptotics profiles, we obtain a quantitative expression for the shape of the film and a relation between the speed of the contact line and the macroscopic and microscopic contact angles.

1 Introduction

The basic equation which describes the spreading of a liquid film – assumed to be uniform in one space direction – along a solid surface is given by

$$h_t + \kappa(h^3 h_{xxx})_x = 0, \tag{1.1}$$

where $h(x,t)$ is the film thickness, t is the time, x the spatial coordinate and $\kappa = \gamma/(3\mu)$, where γ is the surface tension and μ is the viscosity of the liquid. Equation (1.1) is derived on the basis of three assumptions: the applicability of the *lubrication approximation* [2], the *no-slip condition* (vanishing velocity of the fluid at the solid surface), and the applicability of the *Laplace formula* $p = -\gamma K$, where p is the hydrodynamic pressure and K the curvature, approximated by h_{xx}.

The main difficulty in the modelling of thin films is the following: from a straightforward asymptotic expansion near the contact lines, i.e. the boundaries of the spatial support of h, it follows that the film can only be nonexpanding. In other words, accepting the validity of (1.1), *an infinite force is needed to make contact lines advance* (cf. Dussan & Davis [18]).

Several attempts have been made to modify equation (1.1) to describe the dynamics of expanding liquid films. A small, positive *effective slip parameter*, $\beta > 0$, was introduced by several authors [18, 21, 22, 24–27] (see Oron *et al.* [28] for a complete list of references); this correction leads to the modified equation

$$h_t + \kappa\left[(h^3 + \beta h^n)h_{xxx}\right]_x = 0, \tag{1.2}$$

where $1 \leqslant n < 3$ is a constant depending on the slip model under consideration (when

$n = 1$, (1.2) reduces to that derived by Greenspan [21]). We shall hereafter be concerned with this approach, but we also mention a recent proposal by Barenblatt *et al.* [1] of a new model, based on the introduction of a small and autonomous region near the contact lines where the lubrication approximation and the Laplace formula are not necessarily valid.

It is well known that equation (1.2) admits solutions with advancing contact lines if $n < 3$. In particular, after the paper by Bernis & Friedman [8], a series of recent papers has been dedicated to the development of a PDE theory for equations similar to (1.2) (see, for example, [3–11, 15, 19, 23, 29] and references therein). All these papers, except for that by Otto [29], deal with the construction and properties of solutions with zero-contact angle at the contact lines, i.e. $h_x \to 0$ as $h \to 0$. In this context, we observe that this is a free-boundary problem and, since the equation is of fourth order, at a contact line three conditions are expected to be needed to determine a solution uniquely. Two of them are obvious: $h = 0$ and vanishing mass flux, $(h^3 + \beta h^n)h_{xxx} = 0$, but the choice of the third condition is less obvious and could possibly involve the contact angle h_x or the pressure, which is proportional to h_{xx}.

In the present paper, we study equation (1.2), discussing a particular problem which arises if one wants to use the contact angle to formulate the third boundary condition at the contact line. To explain this problem, we need several preliminary observations. It is often the case that the dynamics of thin films is governed by the dynamics of the contact lines, in the sense that, given the position of the contact lines, equilibrium is established in a relatively short period of time in most of the film (i.e. $h_{xxx} \approx 0$ away from the contact lines; as a matter of fact we shall prove that the approximate solutions which we construct in the present paper satisfy this property). Consequently, the profile of most of the film is a parabola, determined by its height (or, almost equivalently, by the position of the contact lines) and the mass of the liquid. This fact makes it possible to define a so-called *effective contact angle*, θ^{eff}, of the film as the angle of the corresponding parabola. Actually, θ^{eff} can be measured using global properties of the film, such as its focal properties (cf. De Gennes [16]). In the literature, empirical laws have been proposed for θ^{eff}, normally written in the form

$$\theta^{\text{eff}} = f(V), \tag{1.3}$$

where f is an empirical function of the speed V of the contact line. In particular, one often encounters for perfect spreading the dynamic law

$$\theta^{\text{eff}} = CV^{\frac{1}{3}} \tag{1.4}$$

for some constant $C > 0$ (where V is thought as a nonnegative quantity; we consider a contact line at the right of the film, cf. Figure 1). Such a relation has also been proposed by Tanner [30] as a first-order approximation for solutions of (1.1).

Now we arrive at the core of the problem. Assuming that equation (1.2) is valid up to the contact line, we need to know how to translate the law (1.4) for the effective contact angle θ^{eff} into a law for the 'real', say *microscopic* contact angle

$$\theta := -h_x(x_c(t), t),$$

where $x = x_c(t)$ is the position of the contact line at the right border of the film (since $|h_x|$

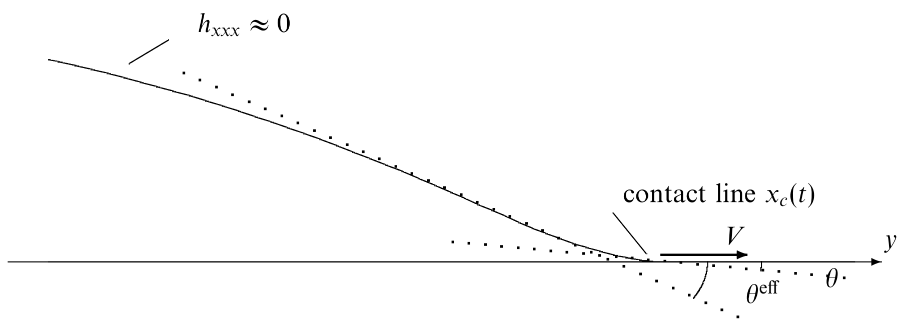

FIGURE 1. Contact angle θ and effective contact angle θ^{eff}.

is assumed to be small in the lubrication approximation, we may identify angles with their tangents). We note that the word microscopic refers to the context of lubrication theory, and is not meant to involve detailed microscopic modelling or molecular dynamics.

Given certain assumptions [25, 14], it is possible to estabilish the relation between θ and θ^{eff} from matched asymptotic expansions. Instead, here we propose to use approximate self-similar solutions, motivated by the fact that, assuming $h(x,t) = t^{\lambda} H(xt^{\lambda})$ – which is the proper scaling for mass conservation – then both equation (1.2) with $\beta = 0$ and condition (1.4) give $\lambda = -1/7$. More precisely, let us consider a solution $h(x,t)$ of equation (1.2) with initially bounded support, and let

$$h(x,t) = t^{-\frac{1}{7}} H(y,t), \qquad y = \frac{xt^{-\frac{1}{7}}}{(7\kappa)^{\frac{1}{4}}};$$

equation (1.2) then transforms into

$$7tH_t - (yH)_y + \left[(H^3 + \beta t^{\frac{3-n}{7}} H^n)H_{yyy}\right]_y = 0. \tag{1.5}$$

Based both on qualitative considerations and on experience with nonlinear diffusion equations, we expect that the term $7tH_t$ will be negligible after a time t_0 of order $\mathcal{O}(\kappa^{-1})$. Hence, we replace (1.5) by

$$\left[(H^3 + \beta t^{\frac{3-n}{7}} H^n)H_{yyy} - yH\right]_y = 0. \tag{1.6}$$

Note that, if $\beta = 0$, then (1.6) would correspond to considering exactly self-similar solutions of (1.2). On the other hand, since

$$H^3 \gg \beta t^{\frac{3-n}{7}} H^n \Longleftrightarrow h^{3-n} \gg \beta,$$

the contribution of $\beta t^{\frac{3-n}{7}} H^n$ will be small on most of the support of H provided

$$\frac{1}{|\{h(\cdot,t) > 0\}|} \int_{-\infty}^{\infty} h^{3-n}(x,t)\, dx \gg \beta; \tag{1.7}$$

therefore, if (1.7) holds then (1.6) corresponds to considering quasi-steady states in the (y,t) variables. In order to analyse (1.6), we assume that

$$t \ll \beta^{-\frac{7}{3-n}}, \tag{1.8}$$

and replace $\beta t^{\frac{3-n}{7}}$ by a positive constant $\varepsilon \ll 1$; thus, we are led to consider the following *model* problem:

$$
\text{(I)}\begin{cases}
\left[(u^3+\varepsilon u^n)u''' - yu\right]' = 0 & \text{in} \quad (-a,a)\\
u>0, \quad u(y)=u(-y) & \text{in} \quad (-a,a)\\
\displaystyle\int_{-a}^{a} u(y)\,dy = 2M & \\
u=0 \quad u' = -\alpha, \quad (u^3+\varepsilon u^n)u'''=0, & \text{at} \quad y=a.
\end{cases}
$$

Here $M>0$, $0<n<3$, $\varepsilon>0$ and $\alpha \geqslant 0$ are given constants, $a>0$ is an unknown constant, and $u(y)$ is an unknown function. We observe that one integration gives

$$\left(u^2+\varepsilon u^{n-1}\right)u''' = y, \quad y\in(-a,a);$$

the equation is therefore degenerate at $u=0$ if $1<n<3$, and singular if $0<n<1$. This implies sensible differences in the mathematical analysis between the two cases: for this reason we shall hereafter restrict ourselves to the physically more relevant case $1 \leqslant n < 3$, though a theory similar to the the one we are going to illustrate could be developed also for $0<n<1$. We also note, in the contexts of numerical simulation and formal asymptotic analysis of thin viscous flows, that comparable approaches have been introduced [12–13, 17, 20], based on the same idea of overcoming the lack of self-similarity via suitable concepts of approximately selfsimilar solutions.

We shall prove for any $M>0$, $1\leqslant n<3$, $\varepsilon>0$ and $\alpha\geqslant 0$ that Problem (I) has a unique solution $(u_{\varepsilon,\alpha}(y), a_{\varepsilon,\alpha})$ (cf. Theorem 2.1), and that for small $\varepsilon>0$ the shape of $u_{\varepsilon,\alpha}(y)$ is a parabola, in the sense that

$$
\left.\begin{aligned}
&\frac{1}{u_{\varepsilon,\alpha}(0)}u_{\varepsilon,\alpha}(a_{\varepsilon,\alpha}r) \longrightarrow 1-r^2 \ \text{ in } C([0,1])\cap C^\infty_{\text{loc}}([0,1))\\
&a_{\varepsilon,\alpha}u_{\varepsilon,\alpha}(0) \longrightarrow \frac{3M}{2}
\end{aligned}\right\} \quad \text{as } \varepsilon\to 0 \tag{1.9}
$$

(cf. Theorem 3.1). Given $\alpha_\varepsilon \geqslant 0$ for $\varepsilon>0$, we may define

$$h_\varepsilon(x,t) := t^{-\frac{1}{7}} u_{\varepsilon,\alpha_\varepsilon}\left(\frac{xt^{-\frac{1}{7}}}{(7\kappa)^{\frac{1}{4}}}\right), \tag{1.10}$$

$$x_c^\varepsilon(t) := (7\kappa)^{\frac{1}{4}} a_{\varepsilon,\alpha_\varepsilon} t^{\frac{1}{7}}, \quad V_\varepsilon := \dot{x}_c^\varepsilon(t); \tag{1.11}$$

note that $h_\varepsilon(\cdot,t)$ are supported in $(-x_c^\varepsilon(t), x_c^\varepsilon(t))$, and

$$\int_0^{a_{\varepsilon,\alpha_\varepsilon}} u_{\varepsilon,\alpha_\varepsilon}(y)\,dy = M \Longleftrightarrow \int_0^{x_c^\varepsilon(t)} h_\varepsilon(x,t)\,dx = \overline{M} = (7\kappa)^{\frac{1}{4}}M. \tag{1.12}$$

Relations (1.9) justify, for small $\varepsilon>0$, the introduction of an effective contact angle $\theta_\varepsilon^{\text{eff}}$ of $h_\varepsilon(x,t)$ as the slope of the corresponding parabola (i.e. the parabola having the same central height $h_\varepsilon(0,t)$ and the same mass $\overline{M}$) at its zero; in other words, since from (1.9) it follows that

$$\frac{h_\varepsilon(x,t)}{h_\varepsilon(0,t)} \sim \left[1-\left(\frac{2h_\varepsilon(0,t)}{3\overline{M}}\right)^2 x^2\right]_+ \quad \text{as } \varepsilon\to 0,$$

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we may define

$$\theta_\varepsilon^{\text{eff}} := \frac{4h_\varepsilon^2(0,t)}{3\overline{M}}, \quad \theta_\varepsilon := -h_{\varepsilon x}(x_c^\varepsilon(t), t). \tag{1.13}$$

Then there exists the following relation between V_ε, $\theta_\varepsilon^{\text{eff}}$ and θ_ε:

$$\frac{\left(\theta_\varepsilon^{\text{eff}}\right)^3 - \theta_\varepsilon^3}{V_\varepsilon \ln \dfrac{1}{\varepsilon}} \longrightarrow \frac{3}{\kappa(3-n)} \quad \text{as } \varepsilon \to 0; \tag{1.14}$$

more precisely (cf. Corollary 4.1), we shall prove that there exists a parameter λ such that for any $\lambda \in [0,1)$ we may choose $\alpha_\varepsilon \geqslant 0$ such that

$$\frac{\theta_\varepsilon}{\theta_\varepsilon^{\text{eff}}} \longrightarrow \lambda \quad \text{as } \varepsilon \to 0 \tag{1.15}$$

and

$$\frac{\left(\theta_\varepsilon^{\text{eff}}\right)^3}{V_\varepsilon \ln \dfrac{1}{\varepsilon}} \longrightarrow \frac{3}{\kappa(3-n)(1-\lambda^3)} \quad \text{as } \varepsilon \to 0. \tag{1.16}$$

In addition, we shall prove that the distance between the contact line $x_c^\varepsilon(t)$ and the zero of the corresponding parabola is indeed small, in the sense that

$$\lim_{\varepsilon \to 0} \frac{x_c^\varepsilon(t) - \dfrac{3\overline{M}}{2h_\varepsilon(0,t)}}{x_c^\varepsilon(t)} = 0. \tag{1.17}$$

Note that, in view of (1.17), we could have almost equivalently defined $\theta_\varepsilon^{\text{eff}}$ as $\theta_\varepsilon^{\text{eff}} = 3\overline{M}/(x_c^\varepsilon(t))^2$: indeed we shall see (cf. Corollary 4.1) that (1.15) and (1.16) continue to hold with this definition. It is also worth remarking that, in proving (1.15)–(1.17), we use neither any hypothesis concerning the parabolic shape of the solution (which instead we prove), nor do we assume any relation between θ^{eff} and V such as (1.3) or (1.4).

Returning to our original equation (1.2), we would like to give an interpretation to (1.14) by setting $\varepsilon = \beta t^{(3-n)/7}$; of course ε is no longer a constant, but on the other hand (1.14) only depends logarithmically on ε. We conjecture that for a large class of solutions of (1.2) the solutions $h_\varepsilon(x,t)$ may be used as intermediate asymptotics, and (1.14) holds for t large enough, but not too large (we recall that the decay rate $t^{-1/7}$ cannot hold for $t \to \infty$, since for very large times the term βh^n in (1.2) becomes dominant with respect to h^3 in all the support of h).

To be more precise we first consider the case of perfect spreading:

$$\theta = 0.$$

Fixing $0 < \beta \ll 1$ and $1 \leqslant n < 3$, let $h_{\beta,n}^0(x,t)$ be a solution of equation (1.2) with mass $2M$ ($\int_{\mathbb{R}} h_{\beta,n}^0(x,t)\,dx = 2M$) and with initially bounded support. The existence of such a solution has been established [3, 10], and it has been proved [5, 6] that for all positive times t the spatial support is a bounded set. Based on the results in these papers we conjecture that, for t large enough, but such that (1.7) and (1.8) hold, $h_{\beta,n}^0(x,t)$ behaves approximately as

$$\frac{3M}{2\tilde{x}_c^3(t)} \left[\tilde{x}_c^2(t) - x^2\right]_+,$$

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where $[s]_+ = \max\{s, 0\}$ and

$$\tilde{x}_c^7(t) = (7\kappa)3^2 M^3 \left(\frac{1}{3-n} \ln \frac{1}{\beta} - \frac{1}{7} \ln t \right)^{-1} t$$

(note that here $\tilde{x}_c(t)$ does not necessarily satisfy $h^0_{\beta,n}(\tilde{x}_c(t), t) = 0$, and represents an 'approximate' contact line). In particular the effective contact angle θ^{eff} and the speed V of the right interface satisfy approximately

$$\frac{(\theta^{\text{eff}})^3}{V} = \frac{3}{\kappa} \left(\frac{1}{3-n} \ln \frac{1}{\beta} - \frac{1}{7} \ln t \right). \tag{1.18}$$

Up to the first order in time, these results reproduce 'Tanner's law'; [30]

$$\tilde{x}_c(t) = c_1 t^{\frac{1}{7}}, \quad \theta^{\text{eff}} = C V^{\frac{1}{3}}.$$

Of course, it is not surprising that $V \to 0$ as $\beta \to 0$ or $n \to 3$.

Concerning solutions with non-zero contact angles we conjecture that for any $\lambda \in (0, 1)$ there exist families of solutions $h^\lambda_{\beta,n}(x, t)$ such that

$$\frac{\theta}{\theta^{\text{eff}}} = \lambda \tag{1.19}$$

and $h^\lambda_{\beta,n}(x, t)$ behaves like

$$\frac{3M}{2\tilde{x}^3_{c,\lambda}(t)} \left[\tilde{x}^2_{c,\lambda}(t) - x^2\right]_+$$

for t large enough but such that (1.7) and (1.8) hold, where

$$\tilde{x}^7_{c,\lambda}(t) = \left(1 - \lambda^3\right) \tilde{x}^7_c(t).$$

In this case we have that, approximately,

$$\frac{(\theta^{\text{eff}})^3}{V} = \frac{3}{\kappa(1-\lambda^3)} \left(\frac{1}{3-n} \ln \frac{1}{\beta} - \frac{1}{7} \ln t \right). \tag{1.20}$$

Using (1.19), (1.18) and (1.20) can be rewritten as

$$(\theta^{\text{eff}})^3 - \theta^3 = \frac{3V}{\kappa} \left[\frac{1}{3-n} \ln \frac{1}{\beta} - \frac{1}{7} \ln t \right]. \tag{1.21}$$

Relations similar to (1.21) have been previously derived through matched asymptotic expansions with a double boundary layer near the contact line. In the radially symmetric case with $n = 2$ and $\theta > 0$, Hocking [25] finds

$$(\theta^{\text{eff}})^3 - \theta^3 = \frac{3V}{\kappa} \left(\ln \frac{1}{\beta} + \ln \frac{\theta r_c(t)}{2e} \right), \tag{1.22}$$

where $r_c(t)$ is the radius of the contact line. In the one-dimensional case, Cox [14] analysed the case of a rough solid surface; if the surface is smooth, his results reduce to

$$g(\theta^{\text{eff}}) - g(\theta) = \frac{3V}{\kappa} \left(\ln \frac{1}{\beta} + \frac{Q_i^*}{f(\theta)} - \frac{Q_0^*}{f(\theta^{\text{eff}})} \right), \tag{1.23}$$

where

$$f(s) = \frac{2 \sin s}{s - \sin s \cos s}, \quad g(s) = 9 \int_0^s \frac{d\zeta}{f(\zeta)} \sim s^3 \quad \text{as } s \searrow 0$$

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and $Q_0^* = Q_0^*(\theta^{\text{eff}}, \frac{d\theta^{\text{eff}}}{dt})$, $Q_i^* = Q_i^*(\theta)$. The lower-order term in (1.21) coincides with the corresponding one in (1.22) if $n = 2$ and $\theta > 0$, and with the corresponding one in (1.23) if $n = 2$. The higher order corrections (for (1.21), $\ln t^{-1/7}$) are different in the three relations; it is not clear whether these differences are real or due to the technique used (i.e. a remnant of the choice of the model problems).

2 The self-similar problem with fixed $\varepsilon > 0$

In this section we discuss the following result:

Theorem 2.1 *Let* $1 \leqslant n < 3$, $\varepsilon > 0$ *and* $M > 0$. *For any* $\alpha \geqslant 0$ *Problem* (I) *has a unique solution* (u_α, a_α), *and the following properties are satisfied:*

(i) $u_\alpha(0)$, $u''_\alpha(0)$ *and* a_α *depend continuously on* α;

(ii)
$$\alpha_1 > \alpha_2 \geqslant 0 \Longrightarrow \begin{cases} u_{\alpha_1}(0) > u_{\alpha_2}(0), \\ a_{\alpha_1} < a_{\alpha_2}; \end{cases}$$

(iii) u_{α_1} *and* u_{α_2} *have exactly one intersection point if* $\alpha_1 \neq \alpha_2$, *i.e. there exists a unique* $y > 0$ *such that* $u_{\alpha_1}(y) = u_{\alpha_2}(y) > 0$;

(iv) $u_\alpha(0) \to \infty$ *and* $a_\alpha \to 0$ *as* $\alpha \to \infty$.

Since the proof of Theorem 2.1 is quite technical and lengthy, we prefer to focus on the proofs of the properties (i)–(iv). For the existence of u_α, which is based on a standard shooting procedure, we only give the main ideas. Introducing the shooting parameters $s > 0$ and $\gamma < 0$, we consider the following initial value problem:

$$(\mathit{II}_{s,\gamma}) \begin{cases} (u^2 + \varepsilon u^{n-1})u''' = y \quad \text{for} \;\; y > 0 \\ u(0) = s, \quad u'(0) = 0, \quad u''(0) = \gamma. \end{cases}$$

By classical ODE theory, for any $s > 0$ and γ problem $(\mathit{II}_{s,\gamma})$ admits a unique maximal solution $u_{s,\gamma} \in C^3([0, a))$, where

$$a = a_{s,\gamma} := \sup\{y \in \mathbb{R}^+ : u_{s,\gamma}(y) > 0\}.$$

In addition there holds:

Claim 1 For any $s > 0$ and γ, and for any sequence $(s_n, \gamma_n) \to (s, \gamma)$ we have

$$u_{s_n,\gamma_n} \longrightarrow u_{s,\gamma} \quad \text{in} \;\; C^3_{\text{loc}}([0, a_{s,\gamma})).$$

Following the ideas of Bernis *et al.* [9], it is possible to prove that:

Claim 2 For all $s > 0$ and $\alpha \geqslant 0$, there exists a unique $\gamma_{s,\alpha} < 0$ and $a > 0$ such that the solution of Problem $(\mathit{II}_{s,\gamma_{s,\alpha}})$ satisfies

$$u > 0 \;\; \text{in} \;\; [0, a), \quad u(a) = 0, \quad u'(a) = -\alpha;$$

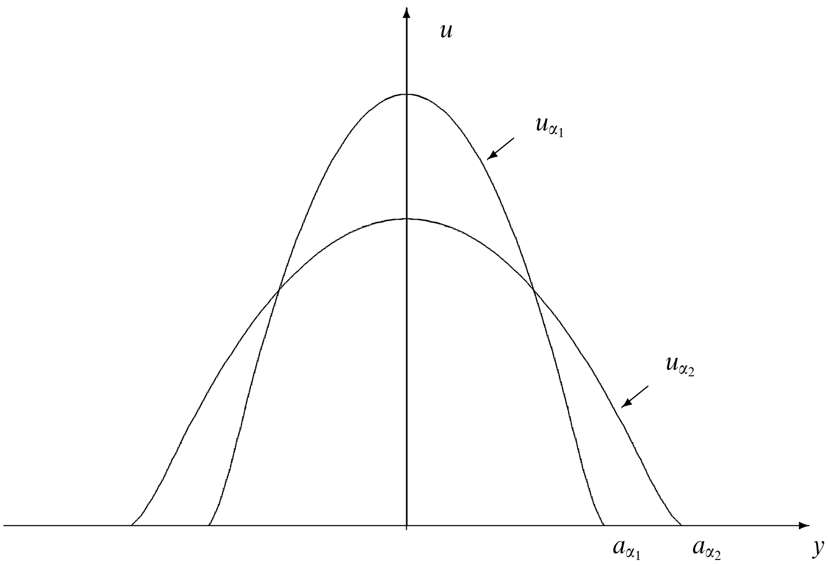

FIGURE 2. Two solutions of Problem I with the same M and ε and with different contact angles: $\alpha_1 > \alpha_2 \geqslant 0$.

Claim 3 For all $M > 0$ and $\alpha \geqslant 0$ there exists a unique $s_M > 0$ such that the solution u of Problem $(\mathit{II}_{s_M,\gamma_{s_M},\alpha})$ satisfies

$$\int_0^a u(y)\,dy = M.$$

Note that $(u^3 + \varepsilon u^n)u'''|_{x=a} = au(a) = 0$, hence the even extension of the solution to $(-a, a)$ is the unique solution of Problem (I).

To prove the remaining part of Theorem 2.1 we need some preliminary results.

Lemma 2.1 *Let $s > 0$ and $\gamma < 0$ be such that the solution $u_{s,\gamma}$ of Problem $(\mathit{II}_{s,\gamma})$ vanishes at some $a > 0$ and is positive in $[0, a)$. If $\overline{\gamma} < \gamma$, then the solution $u_{s,\overline{\gamma}}$ of Problem $(\mathit{II}_{s,\overline{\gamma}})$ vanishes at some $\overline{a} > 0$, is positive in $[0, \overline{a})$ and*

$$\overline{a} < a,$$
$$u_{s,\overline{\gamma}} < u_{s,\gamma} \quad \text{in } (0, \overline{a}],$$
$$u'_{s,\overline{\gamma}}(\overline{a}) < u'_{s,\gamma}(a).$$

Proof Setting $u = u_{s,\gamma}$ and

$$\varphi(u) := u^2 + \varepsilon u^{n-1}, \tag{2.1}$$

we have

$$u''' = \frac{y}{\varphi(u)} \quad \text{if } u > 0, \tag{2.2}$$

whence

$$u'' \nearrow \quad \text{as long as } u \text{ exists and } u > 0. \tag{2.3}$$

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In particular,

$$\left.\begin{array}{l} u > 0 \quad \text{in} \quad [0, a) \\ u(a) = 0 \end{array}\right\} \Longrightarrow u \searrow \quad \text{in} \quad [0, a).$$

Hence we may use u as an independent variable, and the function

$$z(u) := \left(u'(y)\right)^2$$

satisfies the equation

$$z'' = -\frac{2y(u)}{\varphi(u)\sqrt{z}} \quad \text{in} \quad (0, s), \tag{2.4}$$

with boundary conditions

$$z(s) = 0, \qquad z'(s) = 2\gamma. \tag{2.5}$$

Setting $\overline{u} = u_{s,\overline{\gamma}}$, we may use $\overline{u}$ as an independent variable as long as $\overline{u}$ is decreasing and positive. Setting

$$\overline{z}(u) := \left(\overline{u}'(y)\right)^2,$$

$$y_0 = \sup\left\{y > 0 : \overline{u} > 0 \ \text{ and } \ \overline{u}' < 0 \ \text{ in } \ (0, y)\right\},$$

$$s_0 = \overline{u}(y_0^-),$$

we obtain that $\overline{z}$ is well defined in (s_0, s), and

$$\begin{cases} \overline{z}'' = -\dfrac{2\overline{y}(u)}{\varphi(u)\sqrt{\overline{z}}} \quad \text{in} \quad (s_0, s), \\ \overline{z}(s) = 0, \quad \overline{z}'(s) = 2\overline{\gamma}. \end{cases}$$

Since $\overline{\gamma} < \gamma$, $\overline{z} > z$ in a left neighbourhood of s. We claim that

$$\overline{z} > z \quad \text{in} \quad [s_0, s)$$

which implies at once the desired result. Arguing by contradiction, we suppose that

$$\overline{z} > z \quad \text{in} \quad (s_1, s) \quad \text{and} \quad \overline{z}(s_1) = z(s_1)$$

for some $s_1 \in [s_0, s)$. Since $\overline{y}(u) < y(u)$ in (s_1, s), it follows that

$$\overline{z}'' = -\frac{2\overline{y}(u)}{\varphi(u)\sqrt{\overline{z}}} > -\frac{2y(u)}{\varphi(u)\sqrt{z}} = z'' \quad \text{in} \quad (s_1, s).$$

Therefore, since $\overline{z}(s) = z(s)$ and $\overline{z}(s_1) = z(s_1)$, we conclude that $\overline{z} < z$ in (s_1, s), and we have obtained a contradiction. □

The following lemma, which we shall often use in the sequel, gives an *a priori* lower bound for solutions of $(\mathbb{I}_{s,\gamma})$.

Lemma 2.2 *Let A and B be positive constants and let $u \in C^3([0, B)) \cap C([0, B])$ satisfy*

$$\begin{array}{c} u > 0, \ u' \leqslant 0, \ u''' \geqslant 0 \quad \text{in} \quad [0, B) \\ u(0) \geqslant A. \end{array}$$

Then there exists a function $f \in C([0, B])$, which depends only upon A and B, such that

$$u(y) \geqslant f(y) > 0 \quad \text{in} \quad [0, B).$$

For the proof we refer to the appendix.

By Lemma 2.1 and Claim 2, the point

$$a_{s,\gamma} < \infty : \quad u_{s,\gamma} > 0 \ \text{in} \ [0, a_{s,\gamma}), \quad u_{s,\gamma}(a_{s,\gamma}) = 0$$

is well defined for $\gamma \leqslant \gamma_{s,0}$. In addition, the following property holds:

Corollary 2.1 *For all $s > 0$, $a_{s,\gamma}$ depends continuously upon γ for $\gamma \leqslant \gamma_{s,0}$.*

Proof It follows from Lemma 2.1 that $a_{s,\gamma}$ is strictly inceasing with respect to γ. Let $\overline{\gamma} < \gamma_{s,0}$ and suppose by contradiction that

$$a^+ = \lim_{\gamma \to \overline{\gamma}^+} a_{s,\gamma} > a_{s,\overline{\gamma}}.$$

Since $u'_{s,\gamma} \leqslant 0$, by Claim 1 we have

$$u_{s,\gamma}(a_{s,\overline{\gamma}}) \to 0 \quad \text{as} \quad \gamma \to \overline{\gamma}^+$$

in contradiction to Lemma 2.2 ($A = s$, $B = a^+$). On the other hand, Claim 1 immediately implies

$$\lim_{\gamma \to \overline{\gamma}^-} a_{s,\gamma} = a_{s,\overline{\gamma}}, \quad \overline{\gamma} \leqslant \gamma_{s,0},$$

which completes the proof. □

Remark 2.1 Following the ideas of Bernis *et al.* [9], we observe that if $\gamma > \gamma_{s,0}$ the solution $u_{s,\gamma}$ is strictly positive and definitely increasing as $y \to \infty$.

Lemma 2.3 *Let u_1 and u_2 be, respectively, solutions of Problems $(\mathbb{I}_{s_1,\gamma_1})$ and $(\mathbb{I}_{s_2,\gamma_2})$, vanishing at a_1 and a_2. If*

$$s_1 < s_2 \quad \text{and} \quad u'_1(a_1) \leqslant u'_2(a_2)$$

then

$$a_1 < a_2 \quad \text{and} \quad u_1 < u_2 \ \text{in} \ [0, a_1].$$

Proof Let $u_{s,\gamma}$ denote the solution of Problem $(\mathbb{I}_{s,\gamma})$ and let

$$\overline{\gamma} = \sup\{\gamma^\star < 0 : u_{s_1,\gamma} < u_2 \ \ (\text{as long as} \ \ u_{s_1,\gamma} \ \text{exists and is positive}) \ \forall \gamma < \gamma^\star\}$$

By a standard argument (cf. Bernis *et al.* [9]), $\overline{\gamma} \in (-\infty, 0)$, and by continuous dependence $\overline{u} := u_{s_1,\overline{\gamma}}$ vanishes at $\overline{a} \leqslant a_2$. We distinguish three possibilities:

I. there exists $y^\star \in (0, \overline{a})$ such that $\overline{u} < u_2$ in $[0, y^\star)$ and $\overline{u}(y^\star) = u_2(y^\star)$;

II. $\overline{u} < u_2$ in $[0, \overline{a}]$;

III. $\overline{a} = a_2$, $\overline{u}'(\overline{a}) = u'_2(a_2)$ and $\overline{u} < u_2$ in $[0, a_2)$.

In case II one can easily prove that $\overline{u}'(\overline{a}) = 0$, since by Corollary 2.1 $\overline{u}'(\overline{a}) < 0$ and $\overline{a} < a_2$ would contradict the definition of $\overline{\gamma}$. Therefore, it follows from Lemma 2.1 that $a_1 \leqslant \overline{a} < a_2$ and $u_1 \leqslant \overline{u}$ in $(0, a_1)$, the desired result.

The proof is complete if we can exclude cases I and III, since the only possibility left is

$$\overline{a} = a_2, \quad \overline{u}'(\overline{a}) > u'_2(a_2) \ \text{ and } \ \overline{u} < u_2 \ \text{ in } \ [0, a_2),$$

and the result follows from Lemma 2.1. We begin with case I. Setting

$$v = u_2 - \overline{u} \quad \text{and} \quad \Phi(v) = vv'' - \tfrac{1}{2}(v')^2,$$

it follows that $v'(y^\star) = 0$, $\Phi(v(y^\star)) = 0$ and since φ is increasing,

$$(\Phi(v))' = (u_2 - \overline{u})(u_2 - \overline{u})''' = (u_2 - \overline{u})y\left(\frac{1}{\varphi(u_2)} - \frac{1}{\varphi(\overline{u})}\right) < 0 \quad \text{if} \quad u_2 \neq \overline{u}.$$

Since $v > 0$ in $[0, y^\star)$, this implies at once that $\Phi(v) > 0$ in $[0, y^\star)$, i.e.

$$v'' > \frac{(v')^2}{2v} \geqslant 0 \quad \text{in} \quad [0, y^\star).$$

But this is impossible, since $v'(0) = v'(y^\star) = 0$.

It remains to eliminate case III. Arguing as above (with $y^\star$ replaced by a_2), $\Phi(v)$ is decreasing in $(0, a_2)$ and we obtain a contradiction if we prove that

$$\lim_{y \to a_2} \Phi(v(y)) \geqslant 0.$$

Since $v'(y) \to 0$ as $y \to a_2$, it is enough to prove that

$$\lim_{y \to a_2} v(y)v''(y) \geqslant 0.$$

Indeed, this inequality follows at once, since otherwise $v''(y) \to -\infty$ as $y \to a_2$, which is impossible since $v(a_2) = v'(a_2) = 0$ and $v > 0$ in $(0, a_2)$. □

Proof of Theorem 2.1 By Lemma 2.1 and Lemma 2.3,

$$\alpha_1 > \alpha_2 \geqslant 0 \Longrightarrow u_{\alpha_1}(0) > u_{\alpha_2}(0). \tag{2.6}$$

To prove (i) we claim that, as $n \to \infty$,

$$\left.\begin{array}{l} s_n \to s \in (0, \infty) \\ \gamma_n \to \gamma \in (-\infty, 0) \\ a_n < \infty \quad \forall n \\ -u'_{s_n,\gamma_n}(a_{s_n,\gamma_n}) \to \alpha > 0 \end{array}\right\} \Longrightarrow \left\{\begin{array}{l} a_{s,\gamma} < \infty \\ u_{s_n,\gamma_n} \longrightarrow u_{s,\gamma} \quad \text{in} \quad C^3_{\text{loc}}([0, a_{s,\gamma})) \\ a_{s_n,\gamma_n} \longrightarrow a_{s,\gamma} \\ u'_{s,\gamma}(a_{s,\gamma}) = -\alpha. \end{array}\right. \tag{2.7}$$

Claim 1 immediately implies the first two assertions, and Lemma 2.2 yields $a_{s_n,\gamma_n} \to a_{s,\gamma}$. It follows easily from (2.3) that there exist two constants $C > 0$ and $\delta > 0$ such that $u'_{s_n,\gamma_n} \leqslant -C$ if $0 < u_{s_n,\gamma_n} < \delta$, which immediately implies that $u'_{s,\gamma}(a_{s,\gamma}) < 0$. It is now possible to prove that $u'_{s,\gamma}(a_{s,\gamma}) = -\alpha$; since the argument is very similar to the one used in the proof of Lemma 4.8 of Bernis *et al.* [9], we omit it here.

Now we are ready to prove (i) for $\alpha > 0$. Let $\alpha_n \nearrow \alpha > 0$. By (2.6), $u_{\alpha_n}(0) \to \underline{s} \in (0, u_\alpha(0)]$, and extracting a subsequence we may assume that $u''_{\alpha_n}(0) \to \underline{\gamma}$. Mass constraint implies $a_{\alpha_n} \geqslant \underline{a} > 0$ and $\underline{\gamma} < 0$, and we have $\underline{\gamma} > -\infty$ since, by Lemma 2.2, u_{α_n} and u'''_{α_n} are uniformly bounded in $[0, \underline{a}/2]$. Thus, by (2.7), u_{α_n} converges to the solution $\underline{u}$ of Problem $(\mathit{II}_{\underline{s},\underline{\gamma}})$, $a_{\alpha_n} \to a_{\underline{s},\underline{\gamma}} < \infty$ and $\underline{u}'(a_{\underline{s},\underline{\gamma}}) = -\alpha$; hence $\underline{u}$ coincides with the unique solution u_α of Problem (I). In particular, $\underline{s} = u_\alpha(0)$ and $\underline{\gamma} = u''_\alpha(0)$. Repeating the same argument if $\alpha_n \searrow \alpha > 0$, we obtain (i) for $\alpha > 0$.

Arguing by contradiction and proceeding as above, it is not difficult to prove that $u_\alpha(0) \to \infty$ as $\alpha \to \infty$. Using Lemma 2.2 and the constraint of fixed M it follows at once that $a_\alpha \to 0$ as $\alpha \to \infty$ and we have proved (iv).

To prove (iii) for $\alpha_1 > \alpha_2 > 0$, we argue by contradiction and suppose that u_{α_1} and u_{α_2} have at least two intersection points. By (iv) and (2.3) there exists $\alpha_0 > \alpha_1$ such that $a_{\alpha_0} < a_{\alpha_2}$ and u_{α_0} and u_{α_2} have exactly one intersection point. Let

$$\underline{\alpha} = \inf\left\{\alpha^\star \in (\alpha_2, \alpha_0) \text{ such that } \forall\, \alpha \in (\alpha^\star, \alpha_0)\, \exists\, !\, y : u_\alpha(y) = u_{\alpha_2}(y)\right\}.$$

Then $\underline{\alpha} \in [\alpha_1, \alpha_0)$,

$$u_{\underline{\alpha}}(0) > u_{\alpha_2}(0), \qquad a_{\underline{\alpha}} < a_{\alpha_2},$$

and there exists $y_0 \in (0, a_{\underline{\alpha}})$ such that

$$u_{\underline{\alpha}} \geqslant u_{\alpha_2} \quad \text{in} \quad (0, y_0) \quad \text{and} \quad u_{\underline{\alpha}} \leqslant u_{\alpha_2} \quad \text{in} \quad (y_0, a_{\underline{\alpha}}).$$

In addition it follows easily that

$$u'_{\underline{\alpha}}(y_0) < u'_{\alpha_2}(y_0).$$

Indeed, if $u'_{\underline{\alpha}}(y_0) = u'_{\alpha_2}(y_0)$ then $u_{\underline{\alpha}} - u_{\alpha_2}$ has an inflection point at y_0, so $u''_{\underline{\alpha}}(y_0) = u''_{\alpha_2}(y_0)$; but then, by uniqueness, $u_{\underline{\alpha}}(y) = u_{\alpha_2}(y)$ for $y \in [0, a_{\underline{\alpha}})$ and we have obtained a contradiction.

It remains to distinguish the following two situations:

I. There exists $y_1 \in (y_0, a_{\underline{\alpha}})$ such that

$$u_{\underline{\alpha}} < u_{\alpha_2} \quad \text{in} \quad (y_0, y_1), \quad u_{\underline{\alpha}}(y_1) = u_{\alpha_2}(y_1), \quad u'_{\underline{\alpha}}(y_1) = u'_{\alpha_2}(y_1).$$

II. There exists $y_2 \in (0, y_0)$ such that

$$u_{\underline{\alpha}} > u_{\alpha_2} \quad \text{in} \quad (y_2, y_0), \quad u_{\underline{\alpha}}(y_2) = u_{\alpha_2}(y_2), \quad u'_{\underline{\alpha}}(y_2) = u'_{\alpha_2}(y_2).$$

In case I we define $v = u_{\alpha_2} - u_{\underline{\alpha}}$ and $\Phi(v) = vv'' - \frac{1}{2}(v')^2$, arguing as in the proof of Lemma 2.3 we have that $\Phi(v(y_1)) < \Phi(v(y_0))$. On the other hand,

$$\Phi(v(y_1)) = 0 \quad \text{and} \quad \Phi(v(y_0)) = -\tfrac{1}{2}\left(u'_{\alpha_2}(y_0) - u'_{\underline{\alpha}}(y_0)\right)^2 < 0$$

and we have obtained a contradiction. In case II we use u as an independent variable and define

$$z(u) = \left(u'_{\alpha_2}\right)^2 \quad \text{and} \quad \underline{z}(u) = \left(u'_{\underline{\alpha}}\right)^2;$$

since $(z - \underline{z})' = 2(u_{\alpha_2} - u_{\underline{\alpha}})'' < 0$ at $u = u_{\underline{\alpha}}(y_2)$, we have $z > \underline{z}$ in a left neighbourhood of $u_{\underline{\alpha}}(y_2)$ (the first inequality is strict since otherwise u_{α_2} and $u_{\underline{\alpha}}$ would coincide). On the other hand, $\underline{z} > z$ at $u = u_{\underline{\alpha}}(y_0)$, and therefore there exists $u^\star \in (u_{\underline{\alpha}}(y_0), u_{\underline{\alpha}}(y_2))$ such that $z(u^\star) = \underline{z}(u^\star)$ and $z > \underline{z}$ in $(u^\star, u_{\underline{\alpha}}(y_2))$. Arguing as in Lemma 2.3, we obtain $(z - \underline{z})'' > 0$ and again we have found a contradiction.

Using (2.6), (iii) and the mass constraint, (ii) now follows immediately for $\alpha > 0$.

It remains to prove (i) if $\alpha = 0$, and (ii) and (iii) if $\alpha_1 > \alpha_2 = 0$. To prove (i) if $\alpha = 0$, it is enough to take the limit $\alpha \to 0$ and use the monotonicity of $u_\alpha(0)$ and a_α for $\alpha > 0$. Hence also (ii) and (iii) follow at once if $\alpha_2 = 0$. This completes the proof of Theorem 2.1. □

3 The effective contact angle

In this section we prove that the solutions of Problem (I) behave as a parabola for small values of ε:

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Theorem 3.1 *Let $M > 0$, $1 \leqslant n < 3$, $\alpha \geqslant 0$ and $\varepsilon > 0$, and let $(u_{\varepsilon,\alpha}(y), a_{\varepsilon,\alpha})$ denote the unique solution of Problem* (I). Then

$$u_{\varepsilon,\alpha}(0) \longrightarrow \infty \quad \text{and} \quad a_{\varepsilon,\alpha} u_{\varepsilon,\alpha}(0) \longrightarrow \frac{3M}{2} \quad \text{as } \varepsilon \to 0 \tag{3.1}$$

and

$$\frac{1}{u_{\varepsilon,\alpha}(0)} u_{\varepsilon,\alpha}(a_{\varepsilon,\alpha} r) \longrightarrow 1 - r^2 \quad \text{in} \quad C([0,1]) \cap C^\infty_{\text{loc}}([0,1)) \quad \text{as } \varepsilon \to 0; \tag{3.2}$$

the limits in (3.1) and (3.2) are uniform with respect to $\alpha \geqslant 0$.

Theorem 3.1 justifies, for small ε, the introduction of an effective contact angle of $u_{\varepsilon,\alpha}$ as minus the slope of the corresponding parabola at its zero:

$$\left(\alpha^{\text{eff}}\right)_{\varepsilon,\alpha} := \frac{4}{3M} u^2_{\varepsilon,\alpha}(0). \tag{3.3}$$

Remark 3.1 It follows from Theorem 2.1 that for any $S \in [1, \infty]$ and for any $\varepsilon > 0$ there exists $\alpha_\varepsilon \geqslant 0$ such that

$$\frac{u_{\varepsilon,\alpha_\varepsilon}(0)}{u_{\varepsilon,0}(0)} \longrightarrow S \quad \text{as } \varepsilon \to 0. \tag{3.4}$$

Denoting by $\alpha^{\text{eff}}_\varepsilon$ and $\alpha^{\text{eff}}_{\varepsilon,0}$ the effective contact angles of $u_{\varepsilon,\alpha_\varepsilon}$ and $u_{\varepsilon,0}$, i.e.

$$\alpha^{\text{eff}}_\varepsilon := \left(\alpha^{\text{eff}}\right)_{\varepsilon,\alpha_\varepsilon} \quad \text{and} \quad \alpha^{\text{eff}}_{\varepsilon,0} := \left(\alpha^{\text{eff}}\right)_{\varepsilon,0}, \tag{3.5}$$

we find that

$$\frac{\alpha^{\text{eff}}_\varepsilon}{\alpha^{\text{eff}}_{\varepsilon,0}} \longrightarrow S^2 \quad \text{as } \varepsilon \to 0. \tag{3.6}$$

In §4 we shall prove the main result of this paper, which establishes a relation between α_ε and $\alpha^{\text{eff}}_\varepsilon$ in terms of S.

Proof of Theorem 3.1 We first show that

$$u_{\varepsilon,0}(0) \longrightarrow \infty \quad \text{as } \varepsilon \to 0. \tag{3.7}$$

In view of Theorem 2.1 (ii) this implies that

$$u_{\varepsilon,\alpha}(0) \longrightarrow \infty \quad \text{uniformly with respect to } \alpha \text{ as } \varepsilon \to 0. \tag{3.8}$$

To prove (3.7), we argue by contradiction and suppose that there exists $C > 0$ and a sequence $\varepsilon_n \to 0$ such that

$$u_{\varepsilon_n,0}(0) \leqslant C \quad \forall n.$$

Using Lemma 2.2 and the constraint of fixed M, it is straightforward to prove, successively, the following claims: there exist positive constants $C_1, \ldots, C_5$ such that

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(i) $u_{\varepsilon_n,0}(0) \geqslant C_1$;
(ii) $a_{\varepsilon_n,0} \geqslant C_2$;
(iii) $u''_{\varepsilon_n,0}(0) \leqslant -C_3$;
(iv) $u''_{\varepsilon_n,0}(0) \geqslant -C_4$;
(v) $a_{\varepsilon_n,0} \leqslant C_5$.

Passing to a subsequence, we may assume without loss of generality that

$$a_{\varepsilon_n,0} \to a > 0, \quad u_{\varepsilon_n,0}(0) \to s > 0, \quad u''_{\varepsilon_n,0}(0) \to \gamma < 0 \quad \text{as } n \to \infty.$$

Hence $u_{\varepsilon_n,0}$ converges to the unique solution u of Problem ($\mathit{II}_{s,\gamma}$) in which $\varepsilon = 0$ as long as $u > 0$. On the other hand (cf. Bernis *et al.* [9]) $u > 0$ in $[0, \infty)$, and we have found a contradiction.

Since $M > 0$ is fixed, Lemma 2.2 and (3.7) imply that $a_{\varepsilon,0} \to 0$ as $\varepsilon \to 0$, and it follows from Theorem 2.1 (ii) that

$$a_{\varepsilon,\alpha} \longrightarrow 0 \quad \text{uniformly with respect to } \alpha \geqslant 0 \text{ as } \varepsilon \to 0. \tag{3.9}$$

We define

$$v_{\varepsilon,\alpha}(r) = \frac{1}{u_{\varepsilon,\alpha}(0)} u_{\varepsilon,\alpha}(a_{\varepsilon,\alpha} r) \quad \text{for } 0 \leqslant r \leqslant 1. \tag{3.10}$$

Then $v_{\varepsilon,\alpha}$ satisfies

$$\begin{cases} v''' = \dfrac{a^4_{\varepsilon,\alpha}}{u^3_{\varepsilon,\alpha}(0)} \dfrac{r}{v^2 + \varepsilon u^{n-3}_{\varepsilon,\alpha}(0) v^{n-1}} & \text{and } v > 0 \quad \text{for } 0 < r < 1 \\ v(0) = 1, \quad v'(0) = v'''(0) = 0, \quad v(1) = 0. \end{cases}$$

We claim that

$$v''_{\varepsilon,\alpha}(0) \longrightarrow -2 \quad \text{as } \varepsilon \to 0, \quad \text{uniformly with respect to } \alpha \geqslant 0. \tag{3.11}$$

Arguing by contradiction, we suppose that there exist sequences $\varepsilon_n \to 0$ and $\alpha_n \geqslant 0$, and $\gamma \in [0, \infty]$, $\gamma \neq 2$, such that

$$v''_{\varepsilon_n,\alpha_n}(0) \longrightarrow -\gamma \quad \text{as } n \to \infty.$$

Since $a^4_{\varepsilon,\alpha}/u^3_{\varepsilon,\alpha}(0) \to 0$ as $\varepsilon \to 0$, uniformly with respect to $\alpha \geqslant 0$, it follows that, if $\gamma < \infty$,

$$v_{\varepsilon_n,\alpha_n}(r) \longrightarrow 1 - \tfrac{1}{2}\gamma r^2 \tag{3.12}$$

uniformly on compact subsets of $[0, \sqrt{2/\gamma}) \cap [0, 1]$. Since $v_{\varepsilon_n,\alpha_n}(1) = 0$ for any n, γ cannot be smaller than 2. On the other hand, if $2 < \gamma < \infty$, $v_{\varepsilon_n,\alpha_n} \to 0$ in $[\sqrt{2/\gamma}, 1]$, in contradiction with Lemma 2.2. A similar argument excludes the possibility that $\gamma = \infty$, and we have proved (3.11).

Of course (3.2) follows at once from (3.11) and (3.12) (with $\gamma = 2$). To complete the proof of Theorem 3.1 we observe that the second limit in (3.1) follows from (3.10) and (3.2):

$$\int_0^1 v_{\varepsilon,\alpha}(r)\, dr = \frac{M}{u_{\varepsilon,\alpha}(0) a_{\varepsilon,\alpha}} \longrightarrow \int_0^1 (1 - r^2)\, dr = \tfrac{2}{3}$$

as $\varepsilon \to 0$, uniformly with respect to $\alpha \geqslant 0$. □

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4 The main result

In this section we prove our main result which relates effective and microscopic contact angles for small ε.

Theorem 4.1 *Let* $M > 0$, $1 \leqslant n < 3$ *and* $S \geqslant 1$. *Let, for any* $\varepsilon > 0$, $\alpha_\varepsilon \geqslant 0$ *be a given contact angle and let the effective contact angles* $\alpha_\varepsilon^{\text{eff}}$ *and* $\alpha_{\varepsilon,0}^{\text{eff}}$ *be defined by* (3.5). *If*

$$\frac{\alpha_\varepsilon^{\text{eff}}}{\alpha_{\varepsilon,0}^{\text{eff}}} \longrightarrow S^2 \quad \text{as } \varepsilon \to 0, \tag{4.1}$$

then

$$\frac{\alpha_\varepsilon}{\alpha_\varepsilon^{\text{eff}}} \longrightarrow \left(1 - \frac{1}{S^7}\right)^{\frac{1}{3}} \quad \text{as } \varepsilon \to 0. \tag{4.2}$$

In addition, the solution $u_{\varepsilon,0}$ *of Problem* (I) with $\alpha = 0$ satisfies

$$\frac{u_{\varepsilon,0}^7(0)}{\ln(1/\varepsilon)} \longrightarrow \frac{3^5 M^4}{2^7(3-n)} \quad \text{as } \varepsilon \to 0. \tag{4.3}$$

Once Theorem 4.1 is proved, letting $\lambda = (1 - S^{-7})^{\frac{1}{3}}$ and using Theorem 3.1 and Remark 3.1, it is straightforward to draw the following conclusions concerning the approximate solutions $h_\varepsilon(x,t)$ which have been defined in the introduction.

Corollary 4.1 *Let* $M > 0$, $1 \leqslant n < 3$ *and let* $h_\varepsilon(x,t)$, $\theta_\varepsilon^{\text{eff}}$, θ_ε, $x_c^\varepsilon(t)$, V_ε *and* $\overline{M}$ *be defined by* (1.10)–(1.13). *Then for every* $\lambda \in [0,1)$ *there exists* $\{\alpha_\varepsilon\}_{\varepsilon>0}$, $\alpha_\varepsilon \geqslant 0$ *such that*

$$\frac{\theta_\varepsilon}{\theta_\varepsilon^{\text{eff}}} \longrightarrow \lambda, \tag{4.4}$$

$$\frac{\left(\theta_\varepsilon^{\text{eff}}\right)^3}{V_\varepsilon \ln \frac{1}{\varepsilon}} \longrightarrow \frac{3}{\kappa(3-n)(1-\lambda^3)}, \tag{4.5}$$

$$\frac{x_c^\varepsilon(t) - \dfrac{3\overline{M}}{2h_\varepsilon(0,t)}}{x_c^\varepsilon(t)} \longrightarrow 0, \tag{4.6}$$

as $\varepsilon \to 0$; (4.4) *and* (4.5) *continue to hold if* $\theta_\varepsilon^{\text{eff}}$ *is replaced by* $3\overline{M}/(x_c^\varepsilon(t))^2$.

The rest of the section will be concerned with the proof of the theorem.

Remark 4.1 Let $v_\varepsilon(r) := v_{\varepsilon,\alpha_\varepsilon}(r)$ be defined by (3.10) for $0 \leqslant r \leqslant 1$. Since $v_{\varepsilon,\alpha_\varepsilon}$ is decreasing we may use v as an independent variable and introduce

$$w_\varepsilon(v) := \left(v_\varepsilon'(r)\right)^2, \quad r = r_\varepsilon(v). \tag{4.7}$$

Since

$$w_\varepsilon(0) = \frac{{a_{\varepsilon,\alpha_\varepsilon}}^2}{u_{\varepsilon,\alpha_\varepsilon}^2(0)} \alpha_\varepsilon^2,$$

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recalling the definition (3.5) of $\alpha_\varepsilon^{\text{eff}}$ and (3.1), we obtain that

$$\frac{\alpha_\varepsilon}{\alpha_\varepsilon^{\text{eff}}} \sim \frac{1}{2}\sqrt{w_\varepsilon(0)} \quad \text{as } \varepsilon \to 0. \tag{4.8}$$

Therefore, $w_\varepsilon(0)$ turns out to be the relevant quantity to consider in order to prove (4.2).

Proof of Theorem 4.1 Let $w_\varepsilon(v)$ be defined by (4.7). Setting

$$\delta_\varepsilon = \frac{2a_{\varepsilon,\alpha_\varepsilon}{}^4}{u^3_{\varepsilon,\alpha_\varepsilon}(0)} \quad \text{and} \quad \sigma_\varepsilon = \varepsilon u^{n-3}_{\varepsilon,\alpha_\varepsilon}(0), \tag{4.9}$$

w_ε satisfies

$$\sqrt{w}w'' + \delta_\varepsilon \frac{r_\varepsilon(v)}{v^2 + \sigma_\varepsilon v^{n-1}} = 0 \quad \text{for } 0 < v < 1 \tag{4.10}$$

and

$$w(1) = 0, \quad w'(1) = 2v''_\varepsilon(0), \quad w(0) = \frac{a_{\varepsilon,\alpha_\varepsilon}{}^2}{u^2_{\varepsilon,\alpha_\varepsilon}(0)}\alpha_\varepsilon^2. \tag{4.11}$$

In view of Theorem 3.1,

$$w_\varepsilon(v) \to 4(1-v) \quad \text{and} \quad r_\varepsilon(v) \to \sqrt{1-v} \quad \text{in } C^\infty_{\text{loc}}((0,1]) \quad \text{as } \varepsilon \to 0 \tag{4.12}$$

and

$$\delta_\varepsilon u^7_{\varepsilon,\alpha_\varepsilon}(0) \longrightarrow \frac{3^4 M^4}{2^3} \quad \text{as } \varepsilon \to 0. \tag{4.13}$$

Multiplying equation (4.10) by v and integrating, we obtain that

$$-\int_0^1 v\sqrt{w_\varepsilon}w''_\varepsilon\, dv = \delta_\varepsilon \int_0^1 \frac{r_\varepsilon(v)}{v + \sigma_\varepsilon v^{n-2}}\, dv. \tag{4.14}$$

Let us consider the left-hand side of (4.14). Since w_ε is concave in $(0,1)$, there exists a unique $\overline{v}_\varepsilon \in [0,1)$, $\overline{v}_\varepsilon \to 0$ as $\varepsilon \to 0$, such that

$$w_\varepsilon(\overline{v}_\varepsilon) = \max_{[0,1]} w_\varepsilon$$

and we write, integrating by parts,

$$\begin{aligned} -\int_0^1 v\sqrt{w_\varepsilon}w''_\varepsilon\, dv &= -v\sqrt{w_\varepsilon}w'_\varepsilon\Big]_0^1 + \tfrac{2}{3}w_\varepsilon^{3/2}\Big]_0^1 + \int_0^1 \frac{v(w'_\varepsilon)^2}{2\sqrt{w_\varepsilon}}\, dv \\ &= -\tfrac{2}{3}w_\varepsilon^{3/2}(0) + \int_0^{\overline{v}_\varepsilon} \frac{v(w'_\varepsilon)^2}{2\sqrt{w_\varepsilon}}\, dv + \int_{\overline{v}_\varepsilon}^1 \frac{v(w'_\varepsilon)^2}{2\sqrt{w_\varepsilon}}\, dv \\ &=: -\tfrac{2}{3}w_\varepsilon^{3/2}(0) + I_1 + I_2. \end{aligned} \tag{4.15}$$

We claim that

$$I_1 \longrightarrow 0 \quad \text{and} \quad I_2 \longrightarrow \tfrac{16}{3} \quad \text{as } \varepsilon \to 0. \tag{4.16}$$

To prove that $I_1 \to 0$ we may assume that $\overline{v}_\varepsilon > 0$. Setting

$$p = -\ln v, \quad \overline{p}_\varepsilon = -\ln \overline{v}_\varepsilon, \quad \omega_\varepsilon(p) = w_\varepsilon(e^{-p}),$$

$\omega_\varepsilon(p)$ satisfies

$$\begin{cases} \omega'' + \omega' + \delta_\varepsilon \dfrac{r_\varepsilon(e^{-p})}{1+\sigma_\varepsilon e^{p(3-n)}}\omega^{-1/2} = 0 \quad \text{for } \ p > \overline{p}_\varepsilon \\ \omega(\overline{p}_\varepsilon) = w_\varepsilon(\overline{v}_\varepsilon) \to 4 \quad \text{as } \ \varepsilon \to 0 \\ \omega'(\overline{p}_\varepsilon) = 0. \end{cases}$$

Observe that $\omega_\varepsilon' < 0$ in $(\overline{p}_\varepsilon, \infty)$. Since $\omega_\varepsilon'(p) \to 0$ as $p \to \infty$, ω_ε' has an absolute minimum, say at $p_{0\varepsilon}$. We claim that

$$\omega_\varepsilon'(p_{0\varepsilon}) \longrightarrow 0 \quad \text{as } \ \varepsilon \to 0, \tag{4.17}$$

which implies that $I_1 \to 0$:

$$\begin{aligned} I_1 = \int_{\overline{p}_\varepsilon}^{\infty} \frac{(\omega_\varepsilon')^2}{2\sqrt{\omega_\varepsilon}}\,dp &< \ (\min_{p \geqslant \overline{p}_\varepsilon} \omega_\varepsilon'(p)) \int_{\overline{p}_\varepsilon}^{\infty} \frac{\omega_\varepsilon'}{2\sqrt{\omega_\varepsilon}}\,dp \\ &= \left(\sqrt{w_\varepsilon(0)} - \sqrt{w_\varepsilon(\overline{v}_\varepsilon)}\right)\omega_\varepsilon'(p_{0\varepsilon}) \longrightarrow 0 \quad \text{as } \ \varepsilon \to 0. \end{aligned}$$

To prove (4.17) we multiply the equation for ω_ε by ω_ε' and integrate by parts:

$$\begin{aligned} \frac{1}{2}\left(\omega_\varepsilon'(p_{0\varepsilon})\right)^2 \ &= \int_{\overline{p}_\varepsilon}^{p_{0\varepsilon}} \omega_\varepsilon'\omega_\varepsilon'' = -\int_{\overline{p}_\varepsilon}^{p_{0\varepsilon}} (\omega_\varepsilon')^2 - \delta_\varepsilon \int_{\overline{p}_\varepsilon}^{p_{0\varepsilon}} \frac{r_\varepsilon(e^{-p})}{1+\sigma_\varepsilon e^{p(3-n)}} \frac{\omega_\varepsilon'}{\sqrt{\omega_\varepsilon}}\,dp \\ &< \delta_\varepsilon \left(\max_{p \geqslant \overline{p}_\varepsilon} \frac{r_\varepsilon(e^{-p})}{1+\sigma_\varepsilon e^{p(3-n)}}\right)\left(\sqrt{\omega_\varepsilon(\overline{p}_\varepsilon)} - \sqrt{\omega_\varepsilon(p_{0\varepsilon})}\right) \to 0 \quad \text{as } \ \varepsilon \to 0. \end{aligned}$$

To complete the proof of (4.2) we consider I_2. Since, by the concavity of w_ε,

$$w_\varepsilon'(1) \leqslant w_\varepsilon'(v) \leqslant 0 \quad \text{if } \ \overline{v}_\varepsilon \leqslant v \leqslant 1$$

and

$$w_\varepsilon(v) \geqslant \frac{w_\varepsilon(\overline{v}_\varepsilon)}{1-\overline{v}_\varepsilon}(1-v) \quad \text{if } \ \overline{v}_\varepsilon \leqslant v \leqslant 1,$$

and since $\overline{v}_\varepsilon \to 0$ as $\varepsilon \to 0$, it follows from Lebesgue's dominated convergence Theorem and (4.12) that

$$I_2 \to \int_0^1 \frac{16v}{2\sqrt{4(1-v)}}\,dv = \frac{16}{3}.$$

In view of (4.14), (4.15) and (4.16), we have that

$$\lim_{\varepsilon \to 0}\left(\delta_\varepsilon \int_0^1 \frac{r_\varepsilon(v)}{v+\sigma_\varepsilon v^{n-2}}\,dv + \frac{2}{3}w_\varepsilon^{3/2}(0)\right) = \frac{16}{3}. \tag{4.18}$$

Let $\rho > 0$ be a small, fixed number. Then there exists $v_\rho \in (0,1)$ and $\varepsilon_\rho > 0$ such that

$$1-\rho \leqslant r_\varepsilon(v) \leqslant 1 \quad \text{if } \ 0 < \varepsilon < \varepsilon_\rho \quad \text{and } \ 0 \leqslant v \leqslant v_\rho.$$

Setting

$$\int_0^1 \frac{r_\varepsilon(v)}{v+\sigma_\varepsilon v^{n-2}}\,dv = J_1 + J_2 := \int_0^{v_\rho} \frac{r_\varepsilon(v)}{v+\sigma_\varepsilon v^{n-2}}\,dv + \int_{v_\rho}^1 \frac{r_\varepsilon(v)}{v+\sigma_\varepsilon v^{n-2}}\,dv$$

it follows at once that

$$\delta_\varepsilon J_2 \longrightarrow 0 \quad \text{as } \ \varepsilon \to 0.$$

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On the other hand,

$$(1-\rho)\int_0^{v_\rho}\frac{1}{v+\sigma_\varepsilon v^{n-2}}\,dv \leqslant J_1 \leqslant \int_0^{v_\rho}\frac{1}{v+\sigma_\varepsilon v^{n-2}}\,dv \quad \text{if } 0<\varepsilon<\varepsilon_\rho,$$

and, since for all $\rho>0$ fixed,

$$\int_0^{v_\rho}\frac{1}{v+\sigma_\varepsilon v^{n-2}}\,dv = \frac{1}{3-n}\ln\left(\frac{v_\rho^{3-n}+\sigma_\varepsilon}{\sigma_\varepsilon}\right) = \frac{1}{3-n}\ln\frac{1}{\sigma_\varepsilon}(1+o(1)) \quad \text{as } \varepsilon\to 0,$$

we obtain from (4.18) that for all $\rho>0$

$$\limsup_{\varepsilon\to 0}\left(\frac{\delta_\varepsilon}{3-n}\ln\frac{1}{\sigma_\varepsilon}+\frac{2}{3}w_\varepsilon^{3/2}(0)\right) \leqslant \frac{16}{3(1-\rho)},$$

and

$$\liminf_{\varepsilon\to 0}\left(\frac{\delta_\varepsilon}{3-n}\ln\frac{1}{\sigma_\varepsilon}+\frac{2}{3}w_\varepsilon^{3/2}(0)\right) \geqslant \frac{16}{3}.$$

By the arbitrariness of ρ we conclude that

$$\frac{\delta_\varepsilon}{3-n}\ln\frac{1}{\sigma_\varepsilon}+\frac{2}{3}w_\varepsilon^{3/2}(0) \longrightarrow \frac{16}{3} \quad \text{as } \varepsilon\to 0. \tag{4.19}$$

We observe that if $\alpha_\varepsilon=0$, then $w_\varepsilon(0)=0$, and (4.19) becomes, in view of (4.9) and (4.13),

$$\frac{3^4M^4\left(\ln\frac{1}{\varepsilon}+(3-n)\ln u_{\varepsilon,0}(0)\right)}{2^3u_{\varepsilon,0}^7(0)(3-n)} \longrightarrow \frac{16}{3} \quad \text{as } \varepsilon\to 0,$$

and hence we obtain (4.3):

$$\frac{u_{\varepsilon,0}^7(0)}{\ln\frac{1}{\varepsilon}} \longrightarrow \frac{3^5M^4}{2^7(3-n)} \quad \text{as } \varepsilon\to 0.$$

If (4.1) is satisfied, then (cf. (3.4))

$$\frac{u_{\varepsilon,\alpha_\varepsilon}^7(0)}{\ln\frac{1}{\varepsilon}} \longrightarrow \frac{3^5M^4S^7}{2^7(3-n)} \quad \text{as } \varepsilon\to 0,$$

and, by (4.9) and (4.13),

$$\lim_{\varepsilon\to 0}\delta_\varepsilon\ln\frac{1}{\sigma_\varepsilon} = \frac{3^4M^4}{2^3}\lim_{\varepsilon\to 0}\frac{\ln\frac{1}{\varepsilon}}{u_{\varepsilon,\alpha_\varepsilon}^7(0)} = \frac{16(3-n)}{3S^7}. \tag{4.20}$$

We obtain from (4.19) and (4.20) that

$$w_\varepsilon^{3/2}(0) \longrightarrow 8\left(1-\frac{1}{S^7}\right) \quad \text{as } \varepsilon\to 0, \tag{4.21}$$

and (4.2) follows from (4.8) and (4.21). □

5 Conclusions

For the evolution of an expanding liquid film h over a solid surface at intermediate time scales $\mathcal{O}(\kappa^{-1}) \leqslant t \ll \beta^{-\frac{7}{3-n}}$ (β represents the slip coefficient and n depends upon the choice of the slip condition), we have obtained a relation between the effective (macroscopic)

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contact angle θ^{eff}, the microscopic contact angle θ and the speed V of the contact line, and a quantitative expression for the shape of h. More precisely,

$$(\theta^{\text{eff}})^3 - \theta^3 \sim \frac{3V}{\kappa}\left[\frac{1}{3-n}\ln\frac{1}{\beta} - \frac{1}{7}\ln t\right],$$

$$h(x,t) \sim \frac{3M}{2\tilde{x}_c^3(t)}\left[\tilde{x}_c^2(t) - x^2\right]_+,$$

where $[s]_+ = \max\{s, 0\}$ and

$$\tilde{x}_c^7(t) = (7\kappa)3^2M^3\left(1 - \left(\frac{\theta}{\theta^{\text{eff}}}\right)^3\right)\left(\frac{1}{3-n}\ln\frac{1}{\beta} - \frac{1}{7}\ln t\right)^{-1} t$$

The derivation of these formulae has been based on rigorous results concerning the behaviour as $\varepsilon \searrow 0$ of solutions $u(y)$ of the nonlinear ODE

$$\left[\left(u^3 + \varepsilon u^n\right)u''' - yu\right]' = 0$$

(cf. Problem (I) in the introduction). The agreement with previous results by Hocking [25] and Cox [14] – obtained through matched asymptotic expansions – and the self-consistency indicate that solutions of Problem (I) represent a useful tool in the description of the dynamics of thin films.

Appendix A

Proof of Lemma 2.2 Let

$$f(y) := \inf_{u\in\mathscr{C}} u(y),$$

where

$$\mathscr{C} = \left\{u \in C^3([0,B)) \cap C([0,B]) : u(0) \geqslant A \text{ and } u > 0,\ u' \leqslant 0,\ u''' \geqslant 0 \text{ in } [0,B)\right\}.$$

The function f is decreasing and $f(0) = A$, $f(B) = 0$. We claim that

$$f \in C([0,B]).$$

For $y_0 \in (0,B)$, for a contradiction let

$$f^-(y_0) := \lim_{y\to y_0^-} f(y) > \lim_{y\to y_0^+} f(y) =: f^+(y_0);$$

then for all $\varepsilon > 0$ there exists $u_\varepsilon \in \mathscr{C}$ and $\xi_\varepsilon \in (y_0 - \varepsilon, y_0 + \varepsilon)$ such that

$$u_\varepsilon(y_0 - \varepsilon) \geqslant f^-(y_0), \quad u_\varepsilon(y_0 + \varepsilon) \leqslant \frac{f^+(y_0) + f^-(y_0)}{2} \tag{A 1}$$

$$u'_\varepsilon(\xi_\varepsilon) \to -\infty \quad \text{as } \varepsilon \to 0. \tag{A 2}$$

Let now $y_0 < y_1 < y_2 < B$; positivity and monotonicity of u_ε and (A 1) imply that

$$\exists\ \eta_\varepsilon \in (y_1, y_2) : \ u'_\varepsilon(\eta_\varepsilon) \geqslant -\frac{f^+(y_0) + f^-(y_0)}{2(y_2 - y_1)}. \tag{A 3}$$

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Therefore (A 2), (A 3) and monotonicity of u_ε'' yield

$$u_\varepsilon''(y) \to \infty \text{ uniformly in } [y_2, B) \text{ as } \varepsilon \to 0,$$

in contradiction with (A 3) and $u' \leqslant 0$. Hence $f^+(y) = f^-(y)$ in $(0, B)$. By the same argument it follows that $f(y) = f^+(y)$ in $[0, B)$, and therefore $f \in C([0, B))$. Continuity in B is trivial since $0 \leqslant f(y) \leqslant \frac{A}{B}(B - y)$, and the claim is proved.

It remains to show that $f(y) > 0$ in $[0, B)$. If not, let $y_0 < B$ and $\{u_\varepsilon\} \in \mathscr{C}$ such that $u_\varepsilon(y_0) \to 0$ as $\varepsilon \to 0$. Let $y_0 < y_1 < B$; since u_ε is decreasing, there exist $\xi_\varepsilon \in (y_0, y_1)$ and $\eta_\varepsilon \in (\xi_\varepsilon, B)$ such that

$$u_\varepsilon'(\xi_\varepsilon) \to 0 \quad \text{and} \quad u_\varepsilon''(\eta_\varepsilon) \to 0 \quad \text{as } \varepsilon \to 0,$$

and a contradiction follows for ε small enough using the monotonicity of u_ε'' and the inequality

$$A \leqslant u_\varepsilon(0) = u_\varepsilon(\xi_\varepsilon) - u_\varepsilon'(\xi_\varepsilon)\xi_\varepsilon + \tfrac{1}{2}u_\varepsilon''(\zeta_\varepsilon)\xi_\varepsilon^2, \quad \zeta_\varepsilon \in (0, \xi_\varepsilon).$$

□

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