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Variational models for moving contact lines and the quasi-static approximation

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This paper proposes the use of a variational framework to model fluid wetting dynamics. The central problem of infinite energy dissipation for a moving contact line is dealt with explicitly rather than by introducing a specific microscopic mechanism which removes it. We analyze this modelling approach in the context of the quasi-steady limit, where contact line motion is slower than bulk relaxation. We find that global effects enter into Tanner-type laws which relate line velocity to apparent contact angle through the role that energy dissipation plays in the bulk of the fluid. A comparison is made to the dynamics of lubrication equations that include attractive and repulsive intermolecular interactions. A Galerkin-type approximation method is introduced which leads to reduced-dimensional dynamical descriptions. Computations are conducted using these low-dimensional approximations, and a substantial connection to lubrication equation dynamics is found.

1 Introduction

The behaviour of liquids in contact with solids is of considerable theoretical and practical interest [24, 74]. Central to their study is the motion of contact lines, the interface where the liquid, solid, and vapor (denoted L-S-V) phases meet. For perfectly homogeneous substrates, the equilibrium angle θ_e which the liquid-vapor interface makes with the surface can be determined simply by minimizing the total of the three interfacial energies $\gamma_{LS}, \gamma_{SV}, \gamma_{LV}$. This leads to the Laplace-Young condition [5, 24]

$$\gamma_{SV} - \gamma_{SL} = \gamma_{LV} \cos\theta_e \approx \gamma_{LV}\left(1 - \theta_e^2/2\right). \tag{1.1}$$

The approximation for small angles will be used throughout.

The dynamics of moving contact lines is much less clear [24, 26, 48, 51, 95]. The major complication is that the usual no-slip boundary condition at the solid surface can lead to the apparent paradox that an infinite amount of energy is dissipated at the contact line [34, 55, 59]. Numerous solutions to this now infamous problem have been proposed. They include models based on Navier slip [46, 49], generalized Navier slip [85], models with precursor films [24, 30], diffuse interface approaches [38, 57, 80, 81, 84], shear thinning rheology [45, 94], chemical activation theories [2, 16] and atomistic models [39, 47].

Beyond identifying the physical mechanisms that allow motion of the contact line, there is the more practical problem of formulating a *macroscopic* description of the overall

dynamics. It has been noted [26] that different microscopic mechanisms can lead to the same macroscopic picture. The question becomes the following: *Is there a set of universal features which allow us to describe moving contact lines without knowing the microscopic mechanisms at work?*

Since the difficulty in a hydrodynamic description of contact line motion is that energy is not dissipated at a finite rate, every theory of contact line motion has, at its core, some physical process which makes the rate of dissipation finite. Perhaps then it is this rate that entirely characterizes the microscopic process. Of course, it is not so easy to see how this enters into a force-based description. In a energy-based variational framework, on the other hand, energy dissipation can be modelled explicitly. The point of this paper is to develop such a model and investigate its consequences.

Models for the moving contact line have an extensive history. One widely utilized class of macroscopic models are laws which relate the speed of the contact line to other properties of the fluid near the contact line. One of the most frequently cited is the empirical law introduced by Tanner [88]

$$V_c \sim \theta^3. \tag{1.2}$$

A remark is in order about the "apparent" contact angle θ. One point of view [51] is that the equilibrium angle (1.1) always applies at the molecular level, and that a different (apparent) angle is seen near, but not at, the contact line. For example, it is understood that in the lubrication limit, the interface profile $h(x)$ near the contact line has the form $h \sim x[\ln x]^{1/3}$. The apparent contact angle arises by (somewhat arbitrarily) prescribing a macroscopic distance from the contact line at which to measure the slope of this profile [22, 24, 35].

The notion of an apparent contact angle can be made precise in the sense of a mathematical limiting procedure. Voinov [93] and Cox [22, 23] have derived expressions similar to (1.2) through a matched asymptotic analysis (see also Bertsch *et al.* [14] and Hocking & Rivers [54]. The inner problem in this analysis is, roughly speaking, a travelling wave problem of the form $h''' = 1/h^2$, which was thoroughly analyzed by Duffy & Wilson [31]. Eggers & Stone [35] have also analyzed the local problem and have developed model-specific logarithmic corrections to Tanner's law.

Local analyses which make use of the apparent contact angle may not tell the entire story, however. There is a known experimental dependence of Tanner's law on droplet size [62, 79] and external flow field [15]. Theoretical arguments have also reached this conclusion [37, 43]. This suggests that a relation between contact line speed and angle is not sufficient, and that a global theory is necessary.

Many global approaches to modelling wetting dynamics use the equations of continuum fluid mechanics, especially lubrication-type equations. These equations have mathematical singularities exactly when contact lines form [7, 8, 10–13, 36, 96, 98]. It should be emphasized that these singularities are due to the degenerate nature of the equations, and not a divergence in the dissipation of energy of a moving contact line Indeed, if the mobility term in the lubrication equation has the form $h^3 + \epsilon h^2$ appropriate for Navier slip, the degeneracy persists even though the energy dissipation is finite.

A number of approaches to deal with the singularities in degenerate thin film equations have been tried. Precursor films can be introduced artificially [30, 61], which effectively

eliminates the true contact line and makes the problem well-posed. This procedure doesn't cover the case of partially wetting fluids, however, because no information about the equilibrium contact angle is present. Another approach is to appropriately define weak, nonnegative solutions [8, 10]. While mathematically appealing, the uniqueness of solutions in this approach is still an open question. In the same spirit as what is presented here, Otto [76] has studied a lubrication equation (not pertaining to wetting) using variational techniques.

Precursor films can be introduced in a physical way by consideration of intermolecular forces between the fluid and substrate which give rise to disjoining pressure [24, 68, 69, 71, 74, 81]. In the case where both attractive and repulsive forces are present, the equations are entirely well-posed [9], and also have a natural variational interpretation in which all surface energies can be identified. Because of this, these models will serve as a basis for comparison with the theory described in this paper.

It should be pointed out that realistic contact line motion may also involve numerous physical effects whose dynamical implications are not considered here. They include the role of surfactants [19, 58, 59, 66, 67, 83, 91], rough surfaces which induce pinning and hysteresis phenomenon [24, 27, 32] and inertial effects [23, 52]. While all of these may be important for accurate modelling and prediction, we concentrate on only the simplest problem: a pure, partially wetting fluid moving along an ideally flat surface.

The present paper utilizes a variational model, based upon the physically intuitive notion of greatest free energy decrease. In this framework, the singularity in energy dissipation at a moving contact line is transparent, and can be eliminated explicitly. There is some history leading up to this kind of formulation. Indeed, many arguments about the role of energy and its dissipation were present in early works of deGennes [24, 25], although a complete dynamical theory was never proposed. A number of variational characterizations of the dynamics of viscous fluids have emerged in recent years. Hele-Shaw flows have been studied in this context by Otto [75], Almgren & Almgren [1] and Glasner [42]. For wetting flows, analytical bounds for droplet spreading in slip-condition models were obtained by Otto and Giacomelli [41] by variational arguments. Similar analysis was performed by the author [43] for a lubrication equation with intermolecular forces. In a different vein, numerical methods for lubrication-type equations have made use of variational inequalities [3, 4, 21]. This paper takes the next step, which is to use variational techniques not just for analysis, but for the actual *modelling* of the dynamics.

Our focus here will be largely directed at a specific limiting case of the dynamics where relaxation is assumed to dominate in the bulk of the fluid. This is the "quasi-steady" limit, an extension of the often invoked "spherical cap approximation" [19]. This idea has been used by other authors in the study of moving droplets [6, 41, 72, 86] as well as capillary ridges [50, 53]. While this limit is instructive from the point of view of comparing to other theories, we also point out the limitations of this approximation (see § 6.3).

The main results achieved here are:

- A general framework is constructed for dynamical descriptions of fluid wetting processes.
- Relationships to other theories and models are discussed, and computational comparisons are made.

- The role of global effects on contact line dynamics is explained.
- A general approximation procedure for variational models is developed.

This paper is organized as follows. Background information of gradient systems and related variational principles if given in § 2, along with an associated approximation procedure. The application to fluid wetting is detailed in § 3. A discussion of the variational implications of disjoining pressure lubrication equations is made in § 4. An important limiting case is considered in § 5, and comparisons are carried out in the context of reduced-dimension approximations in § 6.

2 Gradient systems and their reduction

At least as far back as Laplace [64] and Young [97], equilibrium fluid mechanics has invoked arguments concerning energy minimization. The dynamical equivalent is that of a *gradient system* (or gradient *flow*; however, here the word flow will only pertain to the motion of a fluid), a class of dynamical systems entirely characterized by an energy functional and an expression which specifies how energy is dissipated. This section collects and summarizes many aspects of gradient system theory, including some philosophy as to their use.

2.1 Mechanical derivation

Lagrangian mechanics can be used to demonstrate the origin of gradient systems. Consider a system whose configuration is given by the generalized coordinates q_i and their time derivatives $\dot{q}_i$. In terms of the Lagrangian $L(q, \dot{q})$, the difference of kinetic and potential energy, the dynamics are given by [63]

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) - \frac{\partial L}{\partial q_j} = -\frac{\partial T}{\partial \dot{q}_j}. \tag{2.1}$$

The dissipation of energy T is regarded as quadratic in $\dot{q}$, and may depend on the q coordinates as well. We can therefore associate with T the symmetric bilinear form

$$T = \frac{1}{2}(\dot{q}, \dot{q})_{g(q)}. \tag{2.2}$$

The "overdamped" case is an important one; it corresponds to ignoring the kinetic energy and the corresponding inertial term in (2.1). In this case the dynamics are given implicitly by

$$\frac{1}{2}\frac{\partial}{\partial \dot{q}_j}(\dot{q}_j, \dot{q}_j)_{g(q)} = -\frac{\partial F}{\partial q_j} \tag{2.3}$$

where $F(q)$ is the potential energy.

To be more general, a system's configuration $\phi(t)$ will lie on a differentiable manifold $\mathscr{M}$ which has a tangent space T_ϕ at ϕ. With $F(\phi)$ representing an energy functional on

$\mathscr{M}$, the corresponding version of (2.3) is the weak differential equation

$$(\phi_t, \psi)_{g(\phi)} = -\langle \delta F, \psi \rangle, \quad \text{for all } \psi \in T_\phi. \tag{2.4}$$

The $<,>$ notation refers to the action of the first variation of the energy as an element of the dual of the tangent space. In other words, it is the change in energy for a perturbation ψ. Note that the energy is guaranteed to decrease:

$$\frac{dF}{dt} = \langle \delta F, \phi_t \rangle = -(\phi_t, \phi_t)_{g(\phi)} \leqslant 0. \tag{2.5}$$

Another way of thinking about the dissipation expression $(\cdot, \cdot)_g$ is as a metric tensor on $\mathscr{M}$. In this sense, (2.4) is just a weak version of the more familiar

$$\phi_t = -\nabla_g F(\phi) \tag{2.6}$$

where ∇_g is the gradient with respect to the geometry induced by the metric g.

2.2 Related variational principles

A different and sometimes more useful characterization of (2.4) is as the minimizer of the variational problem

$$\phi_t = \Phi : \ \Phi \text{ minimizes } \frac{1}{2}(\Phi, \Phi)_{g(\phi)} + \langle \delta F(\phi), \Phi \rangle. \tag{2.7}$$

This statement can be paraphrased as a physical principle:

> "A system's free energy decreases as quickly as possible subject to a penalty of energy dissipation." (P1)

Numerous physical models have the form of a gradient system [18, 60, 78, 90]. It has been recently realized that viscous fluid mechanics can fit into this framework, including porous media flows [77], Hele-Shaw flows [42, 75], and lubrication models [44, 76].

In the context of hydrodynamical motions, there is more to be said about the variational principle (P1). Suppose that a system's free energy is a function of the Eulerian configuration (for incompressible fluids, this is just the volume the fluid occupies) but does not depend on the Lagrangian positions of individual molecules. Then there may be many trajectories the system can take which each reduce the free energy by the same amount. In this case, the second half of (P1) can be invoked, requiring the selected trajectory to be the one with the least dissipation.

This fact is illustrated by the dynamics of a viscous, inertialess fluid given by Stokes' equations. It is well known that these equations formally minimize the the viscous energy dissipation, subject to conditions which fix the velocity on the boundary. This amounts to a second physical principle

> "For a given change in configuration, the fluid flow is such that the energy dissipation is least." (P2)

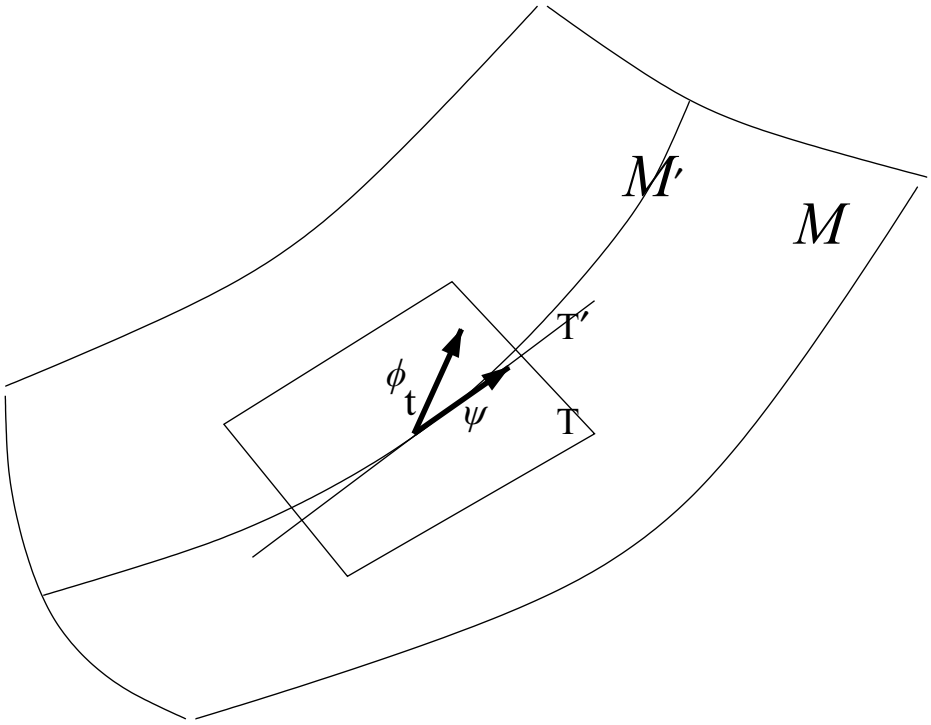

FIGURE 1. Schematic representation of the approximating manifold M' and its corresponding tangent space T'.

This idea is behind some intriguing connections [42, 75, 76] which can be made between fluid mechanics and the problem of optimal mass transport [17, 40, 70, 92].

2.3 A Galerkin reduction method

To make progress using (2.4), a dimensional reduction procedure will be employed. The idea is to approximate solutions by functions of a finite set of time-dependent variables

$$\phi = \Phi(x; p_1(t), p_2(t), \dots, p_n(t)). \tag{2.8}$$

The variables $p_1, p_2, \dots$ parameterize a submanifold $\mathscr{M}'$ of $\mathscr{M}$. In contrast to standard Galerkin methods, this submanifold needn't be a linear subspace.

The dynamics of $p_i(t)$ are generated by restricting the gradient system to this submanifold. This is equivalent to computing the minimizer of (2.7) with the constraint that ϕ_t lies in the tangent space of the approximating submanifold (see Figure 1). This formally yields the finite-dimensional system

$$-A(p)p_t = -\nabla_p F(\Phi(p)) \tag{2.9}$$

where $p = (p_1, p_2, \dots)^T$ and $A(p)$ is the symmetric matrix with components

$$A_{ij} = \left(\frac{\partial \Phi}{\partial p_i}, \frac{\partial \Phi}{\partial p_j}\right)_{g(\Phi(p))}. \tag{2.10}$$

This reduction procedure is also suitable for "infinite-dimensional" approximations. In § 5, we consider an ansatz which parameterizes the fluid's configuration in terms of the contact line shape alone.

Why is the restriction of the gradient system to the approximating manifold a good approximation? It turns out that this is just the orthogonal projection (with respect to the inner product g) of the actual dynamics ϕ_t onto the tangent space $T'(\phi)$ of the approximating manifold. In other words, the approximation is the best is the sense that the "error"

$$\varepsilon(\psi) = (\phi_t - \psi, \phi_t - \psi)_{g(\Phi(p))}, \tag{2.11}$$

is minimized over all $\psi \in T'(\phi)$ when $\psi = \nabla_p \Phi(p) \cdot p_t$, where p_t is defined in (2.9). This can be demonstrated formally as follows. The time derivative of $\Phi(p(t))$ is just $\nabla_p \Phi(p) \cdot p_t$ which means that the tangent space T' is just the range of the linear operator $\nabla_p \Phi(p) : \mathbb{R}^n \to \mathscr{M}$. Suppose $\psi^* \in T'(\phi)$ is the minimizer of ε. Any perturbation $\psi' \in T'(\phi)$ about this minimum leaves the variation stationary, that is

$$(\phi_t - \psi^*, \psi')_{g(\Phi(p))} = 0, \quad \forall \psi' \in T'(\phi), \tag{2.12}$$

which is the same as saying that $\phi_t - \psi^*$ is orthogonal to all of $T'(\phi)$, with respect to the inner product g. Using (2.4) and (2.12),

$$(\psi^*, \psi')_{g(\Phi(p))} = (\phi_t, \psi') = -\langle \delta F, \psi' \rangle, \quad \forall \psi' \in T'(\phi), \tag{2.13}$$

which is a gradient system restricted to T'. Using the basis elements $\{\partial \Phi / \partial p_i\}_{i=1,\ldots,n}$ as test functions ψ' in this expression gives the system (2.9)–(2.10).

A practical implementation of this method requires some analytic information in order to form a suitable ansatz (2.8). This could be obtained, for example, by either physical assumptions or asymptotic methods. In any case, for the ansatz (2.8) to be reasonable, it should be expected that arbitrary initial data will be (approximately, at least) attracted to this solution. In this sense, the method presented here is in the same spirit of nonlinear Galerkin numerical methods [65, 73] which rely on the existence of an exponentially attracting "inertial manifold".

3 Variational formulation

We now explain how to use (2.4) as the mathematical basis for inertialess wetting fluid flows. For ease of presentation, we shall focus on the lubrication limit, where the fluid's free surface height is given by the graph $h(x, y, t)$ and the small angle approximation in (1.1) applies. The support of h will be denoted by Ω, and the contact line Γ will be defined as the boundary of Ω. We will suppose that h is sufficiently differentiable and correctly describes the fluid's configuration up to a microscopic scale near the contact line. In doing this, we are deliberately ignoring the fluid structure at the contact line. The physics of the dynamic contact line will be described entirely by the energy dissipated there.

As pointed out in the introduction, the definition of the apparent contact angle can be somewhat ambiguous. In fact, this concept is not essential to the model developed here. On the other hand, such a definition is useful for two reasons. The first is mathematical

convenience; we shall see that certain calculations simplify by introducing this variable. The second is a desire to compare with existing theories and experiments which make explicit reference to an apparent contact angle. Because of the assumed differentiability of h, in the small-angle limit we can explicitly define

$$\theta = -\frac{\partial h}{\partial n}, \quad n = \text{outward normal to } \Gamma. \tag{3.1}$$

Because h is a macroscopic quantity which does not necessarily describe what happens *at* the contact line, this definition of apparent contact angle should be perceived as an extrapolation of the free surface shape in the bulk, and not the "local" or "microscopic" contact angle.

3.1 Energy and viscous dissipation

A fluid's free energy is the sum of surface energies and body forces (e.g. see Dietrich & Napiorkowski [29] and Israelachvili [56]). This results in an energy functional for the free surface height h

$$E(h) = \int_\Omega \gamma_{SL} - \gamma_{SV} + \gamma_{LV}\left(1 + \frac{1}{2}|\nabla h|^2\right) + \Phi(h, x)\, dx. \tag{3.2}$$

The term multiplying the liquid-vapor energy is the linearized contribution of surface area of the free surface. Φ is a potential associated with bulk energies of the fluid such as gravity. While Φ may also incorporate microscopic energies, such as those associated with van der Waals forces, we will assume that these have been accounted for already in the surface energy terms.

The functional (3.2) forms one component of the variational model; the other is a specification of a bilinear form $(h_t, h_t)_{g(h)}$, representing the dissipation of energy associated with a given motion h_t. In the lubrication limit [20], assuming no fluid slip along the solid, the fluid velocity u is horizontal and is given by

$$\mu u = \left(zh - \frac{z^2}{2}\right)\nabla p \tag{3.3}$$

where z is the vertical coordinate and μ is the viscosity. The corresponding flux of material is

$$J = \int_0^h u\, dz = -\frac{h^3}{3\mu}\nabla p. \tag{3.4}$$

The energy dissipated is a result of horizontal viscous shear only, and is therefore [5]

$$D = \mu \int_\Omega \int_0^h |u_z|^2\, dz\, dx = 3\mu \int_\Omega \frac{J^2}{h^3}\, dx. \tag{3.5}$$

The flux is related to the time derivative of h by the continuity equation and no-flux boundary condition

$$h_t + \nabla \cdot J = 0, \quad J|_{h=0} = 0. \tag{3.6}$$

Given h, h_t, the flux can be found by solving (3.4,3.6) together. It is in this way that equation (3.5) specifies a bilinear form on h_t.

Conversely, consistent with variational principle (P2), J formally minimizes D subject to the constraint $h_t = -\nabla \cdot J$. Because the constraint is linear, an admissible perturbation δJ of J satisfies $\nabla \cdot \delta J = 0$. The variation of D is stationary with respect to such perturbations, so

$$\int_\Omega \frac{J \cdot \delta J}{h^3}\, dx = 0, \tag{3.7}$$

for all $\nabla \cdot \delta J = 0$. This is equivalent to saying that J/h^3 is orthogonal to all divergence-free vector fields, which according to the Helmholtz decomposition means that $J/h^3 = -\nabla \Pi$ where Π is some scalar function. Since J satisfies (3.6), J is found according to

$$J = -h^3 \nabla \Pi, \quad \nabla \cdot (h^3 \nabla \Pi) = h_t \tag{3.8}$$

subject to no-flux boundary conditions at the droplet edge. Notice that in (3.8), $3\mu\Pi$ can be regarded as the physical pressure in (3.3).

3.2 The stress singularity and modifications of the energy dissipation

Since the energy and dissipation are completely specified by (3.2) and (3.5), the dynamics should follow from (2.4). Unfortunately, a rather severe problem arises in computing (3.5). Suppose that $x = Vt$ designates the moving contact line at time t, and assume that h has a regular expansion near this point

$$h = \theta(x - Vt) + \mathcal{O}((x - Vt)^2), \quad x - Vt \geqslant 0. \tag{3.9}$$

The associated (one-dimensional) flux can be found by solving $-J_x = h_t$ together with a no-flux condition at the line itself, which leads to

$$J \sim Vh \sim V\theta(x - Vt). \tag{3.10}$$

Computing the local energy dissipation involves an integral like

$$\int \frac{J^2}{h^3} \sim \int \frac{V^2}{\theta z}\, dz, \quad z = x - Vt, \tag{3.11}$$

which diverges logarithmically at the contact line $z = 0$. This is the famous singularity found by Huh & Scriven [55], and is the crux of the moving contact line problem.

By altering the way in which energy dissipation is specified, a well-posed notion of contact line dynamics can be obtained as a gradient system with energy (3.2) and inner product given as the modified version of the bilinear expression (3.5). As mentioned earlier, there are numerous possibilities for the mechanisms which mediate contact line motion. Correspondingly, there are many ways in which the logarithmic singularity in (3.5) can be alleviated. It is reasonable to imagine that the energy dissipation should only be modified near the contact line; in the bulk of the fluid, viscous dissipation is bounded

and is assumed to be consistent with the specification of Newtonian stresses (this could of course be altered for the case of other rheologies). We therefore set

$$D = 3\mu \int_{\Omega_\epsilon} \frac{J^2}{h^3}\, dx, \quad \Omega_\epsilon = \{x | h \geqslant \epsilon\}, \tag{3.12}$$

where ϵ is some microscopic scale. To be very general, one should not imagine that ϵ is necessarily constant (it could be, for example, dependent on the solid properties or local fluid configuration). On the other hand, as long as the energy dissipated at the contact line is bounded, *we can always define ϵ so that (3.12) is the exactly the energy dissipated in any particular physical situation.*

It is quite another question to determine ϵ from microscopic physics. We shall take the simplest course, which is to regard ϵ as a constant. Numerical experiments in section 6 lend some justification to this assumption.

4 The relationship to lubrication equations

The purpose of this section is to draw a connection between the variational model and a particular class of PDE's which describe wetting dynamics in a well-posed fashion. We shall see that many features are similar between the two approaches, so that their dynamics are in many cases comparable. Numerical experiments in § 6 will be used to make quantitative comparisons.

As long as $h > 0$, the energy dissipation expression (3.5) has no singularities at all, and can be written using (3.8) as

$$D(h_t, h_t) = -3\mu \int (\Pi) h_t\, dx, \quad \nabla \cdot (h^3 \nabla \Pi) = h_t. \tag{4.1}$$

Invoking (2.4), this leads to

$$\int (3\mu\Pi - \delta E)\psi\, dx = 0 \tag{4.2}$$

for all "admissible" ψ. Since ψ represents a perturbation of h, mass conservation implies that integral of ψ is zero. Therefore $3\mu\Pi - \delta E$ is orthogonal to functions having zero integral, which means that it is equal to a constant. Using the definition of Π, the evolution of h is therefore

$$h_t = \frac{1}{3\mu} \nabla \cdot (h^3 \nabla \delta E), \tag{4.3}$$

which represents a general class of lubrication equations.

For the case of partial wetting (positive equilibrium contact angle) in particular, information about the solid-liquid and solid-vapor surface energies must be included in E. This can be done using disjoining pressure models [9, 24, 68, 69, 74, 81] which include solid/liquid intermolecular interactions. In their most basic form, they fit into the

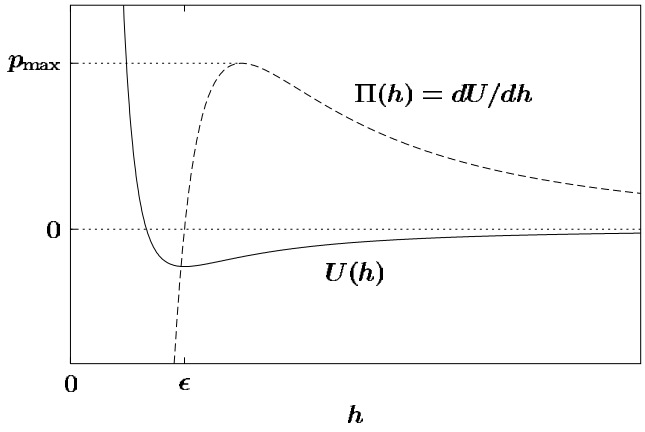

FIGURE 2. Sketch of the intermolecular potential $U(h)$ and the disjoining pressure $\Pi(h) = dU/dh$.

variational template (4.3) with energy

$$E(h) = \int U(h) + \gamma_{LV} \left(1 + \frac{1}{2}|\nabla h|^2\right) dx, \tag{4.4}$$

and dissipation which is identical to (3.5). (In fact, many lubrication-type equations have a variational counterpart [41, 44, 76, 81]. Whereas the potential $U(h)$ can take many different forms [56], we shall take the view that only the qualitative shape is important in the discussion that follows. In particular, it is supposed that

(1) U has a global minimum at ϵ

(2) $U'(h) \to 0$ as $h \to \infty$

(3) $U \to \infty$ as $h \to 0$.

Figure 2 shows the graph of such a function.

The introduction of such a potential precludes any true contact line in the lubrication equations dynamics [9]. This can be seen on the basis of energetic reasoning: if $h \to 0$, $U(h)$ would become very large, leading to an unphysical increase in energy. On the other hand, a film of nominal thickness $\mathcal{O}(\epsilon)$ may be thought of as effectively "solid". In this way, the contact line is really a diffuse but coherent structure which connects this film to the bulk fluid.

The formal limit $\epsilon \to 0$ corresponds to a situation where the precursor region becomes the solid-vapor interface, and the transition region vanishes. In this sense, the various surface energies can be identified in the disjoining pressure model. A flat film of macroscopic thickness $h \gg \epsilon$ will have an energy density which is the sum of liquid-vapor and liquid solid surface energy γ_{LS}

$$\gamma_{LS} + \gamma = E(h \gg \epsilon) = U(\infty) + \gamma \tag{4.5}$$

Alternatively, a film of thickness $h = \epsilon$ representing an essentially dry surface will have the solid-vapor energy γ_{SV}, so that

$$\gamma_{SV} = E(\epsilon) = U(\epsilon) + \gamma. \tag{4.6}$$

Subtracting (4.5) and (4.6) gives a relationship between the potential and surface energies

$$\gamma_{SL} + \gamma - \gamma_{SV} = U(\infty) - U(\epsilon). \tag{4.7}$$

In addition to the first three properties, suppose that $U = U(h;\epsilon)$ is chosen in such a way that

(1) Equation (4.7) holds for all ϵ.

(2) $U(h) \to 0$ as $\epsilon \to 0$ for all $h > 0$.

An example of a function which satisfies all the necessary requirements is given in § 6. With these assumptions in place, the disjoining pressure model's energy converges to that of the variational model (3.2).

In contrast, it is not so easy to see what effect finite ϵ has on the dissipation of energy. The expression (3.5) applies equally to the variational model as well as the lubrication equation. On the other hand, the flux J and free surface profile h are not identical in these different models, which implies two possible sources for discrepancy:

- The structure of h near the contact line is different in the two models, which can potentially affect the integrand in (3.5). On the other hand, if the dissipation contribution is unimportant there, it suffices to only consider the dissipation in the bulk where $h \gg \epsilon$, akin to the cutoff regularization introduced for the variational problem. This idea is favorably verified by the numerical experiments in section (6.1).
- Since the contact line structure is diffuse, the no-flux boundary condition for the variational model doesn't directly apply. If we suppose that near the (one-dimensional) diffuse contact line the motion is that of a travelling wave $h \sim h(x - Vt)$, then the conservation law $h_t + J_x = 0$ reads $-Vh_x = J_x$. With the boundary conditions $h(+\infty) = \epsilon$ and $J(+\infty) = 0$, this equation integrates to

$$J = V(h - \epsilon). \tag{4.8}$$

  This may be contrasted for the result (3.10) for the sharp contact line. While the results differ essentially by a factor of $O(\epsilon)$, this can amount to a substantial change in the nearly singular integrand of (3.5). This difference is apparent in the computations of § 6.2.

5 The quasi-static limit

We will now examine a certain limiting case of the dynamics which proves to be instructive in understanding the consequences of the variational model. The situation to be considered is where the internal part of a fluid droplet relaxes much faster than the contact line moves, so that the droplet's shape is approximately determined by minimizing the energies subject to the constraint of a fixed contact line. Dynamically speaking, this means that the set of quasi-steady droplet shapes forms an approximate inertial manifold, and the ideas of § 2.3 can be invoked. Of course, for arbitrary initial data, there may be a transient period of time in which the solution is not close to this manifold, and the approximation would be invalid.

5.1 Dimensionless form

To be more precise about the when the quasi-static limit applies, a dimensional analysis will be carried out. It should be emphasized that this limit is not exactly the same as the limit of small capillary number considered elsewhere [22]. The reason is that in contrast to a local analysis, the global problem has an additional non-dimensional quantity, the aspect ratio.

Let W, H be the typical scales for width and height of a droplet. There are two velocity scales: V_l, the intrinsic contact line velocity, and $V_c = \gamma_{LV}/3\mu$, the capillary velocity. In the fluid bulk, capillary relaxation will proceed according to the lubrication equation

$$h_t = \frac{1}{3\mu}\nabla \cdot (h^3 \nabla[-\gamma_{LV}\Delta h + d\Phi/dh]), \tag{5.1}$$

which can be non-dimensionalized by rescaling

$$x = Wx'; \quad h = Hh'; \quad t = \tau_c t', \quad \Phi'(h') = \alpha^2 \Phi(Hh')/\gamma_{LV} \tag{5.2}$$

where $\alpha = H/W$ is the aspect ratio and τ_c is a characteristic timescale we are free to choose. Insisting that the non-dimensional equation be free of parameters indicates the choice

$$\tau_c = \frac{W^4}{H^3} V_c \tag{5.3}$$

which gives, after dropping primes,

$$h_t = \nabla \cdot (h^3 \nabla[\Delta h + d\Phi/dh]). \tag{5.4}$$

The timescale for contact line movement is, with respect to the same rescaling

$$\tau_l = \frac{W}{V_l}. \tag{5.5}$$

For capillary relaxation to dominate, one needs $\tau_c \ll \tau_l$, which is equivalent to

$$\frac{V_l}{V_c} \ll \alpha^3. \tag{5.6}$$

Therefore it is only important that the capillary number V_l/V_c be small *relative* to the aspect ratio. In § 6.3, an example is discussed which does not satisfy this condition.

We can proceed to rescale in the variational context as well. The non-dimensional energy is $E' = \gamma_{LV}/H^2$ and the non-dimensional dissipation is $D' = DH\tau_c/(3\mu W^4)$. We can also define a rescaled equilibrium contact angle and cutoff as

$$\theta_e' = \theta_e/\alpha, \quad \epsilon' = \epsilon/H. \tag{5.7}$$

The primes will be dropped hereafter. Using (1.1) energy and dissipation can be written

$$E = \int_\Omega \frac{1}{2}\left(\theta_e^2 + |\nabla h|^2\right) + \Phi(h)\, dx, \tag{5.8}$$

and

$$D = \int_{\Omega_\epsilon} \frac{J^2}{h^3}\, dx, \quad \Omega_\epsilon = \{x | h \geqslant \epsilon\}. \tag{5.9}$$

5.2 Dynamics in the quasistatic limit

Many studies [2, 14, 16, 22–24, 33, 88] propose a relationship between the apparent contact angle (suitably defined, of course) and the velocity of the form $V = V(\theta, \theta_e)$. In this section, this type of approximation will be sought in our model. It will be shown that a local relationship between speed and contact angle is only true to leading order. Corrections to this relationship are significant, in particular they are:

- Only weakly (i.e. logarithmically) separated from the leading-order term.

- Non-local: they do not merely depend on what is happening near the contact line, but rather involve the overall fluid geometry and flow.

Suppose that a droplet has support Ω, and Γ, the boundary of Ω, designates the contact line. A quasi-static droplet's shape is specified entirely by the contact line Γ since it is the minimizer of (3.2), subject to the constraints of constant mass and a fixed contact line. This amounts to solving the problem

$$-\Delta h + \frac{d\Phi}{dh} = \lambda, \quad h|_\Gamma = 0, \quad \int h\, dx = M \equiv \text{volume}, \tag{5.10}$$

where λ is a Lagrange multiplier. In this sense, Γ parameterizes an approximation of the fluid configuration, and according to the ideas of § 2.3, we can obtain a dynamical approximation just by considering the gradient system with Γ as the configuration variable. This requires us to compute the change in energy and the energy dissipated corresponding to any deformation of Γ. It is important to mention that when $\Phi \neq 0$, the solution of (5.10) may be unphysically negative. For now we ignore that possibility.

Let $\delta\Gamma$ represent an arbitrary normal perturbation to the curve Γ, and let δh be the corresponding change in h. The apparent contact angle is given by (3.1) as the inward normal derivative of h. A variation of (5.8) with respect to δh gives the change in energy

$$\langle \delta E, \delta\Gamma \rangle = \int_\Gamma \left(\theta_e^2/2 + \theta^2/2\right) \delta\Gamma\, ds + \int_\Omega \nabla h \cdot \nabla \delta h + \frac{d\Phi}{dh} \delta h\, dx. \tag{5.11}$$

The change in h at the boundary is related to the change in the boundary location itself by $\delta h|_\Gamma = \theta \delta\Gamma$. Using (5.10) and Green's theorem,

$$\begin{aligned} \int_\Omega \nabla h \cdot \nabla \delta h + \frac{d\Phi}{dh} \delta h\, dx &= \int_\Omega \left(-\Delta h + \frac{d\Phi}{dh}\right) \delta h\, dx - \int_\Gamma \theta^2 \Gamma\, ds \\ &= \lambda \int_\Omega \delta h\, dx - \int_\Gamma \theta^2 \delta\Gamma\, ds. \end{aligned} \tag{5.12}$$

Conservation of mass implies that the integral of δh is zero. Combining (5.11) and (5.12) gives

$$\delta E = \int_\Gamma (\theta_e^2/2 - \theta^2/2)\delta\Gamma \, ds. \tag{5.13}$$

The dissipation expression (5.9) is more difficult to compute, since explicit solutions for the flux (3.8) are not readily obtained. Because of the near-singularity, however, the contribution of (5.9) near the moving contact line is much larger than in the bulk of the fluid, and so it is possible to extract the leading-order behaviour by just a local analysis. Let (r, s) be a moving, orthogonal coordinate system fitted to the boundary Γ, where r is the distance from Γ. Let η be an intermediate length scale satisfying $\epsilon \ll \eta \ll 1$, and let $z = r/\eta$ be a rescaled normal coordinate. Derivatives with respect to t are computed via the chain rule in the new coordinates:

$$\frac{\partial}{\partial t} \to \frac{\partial}{\partial t} + \eta^{-1}\frac{\partial}{\partial z}r'(t) + \frac{\partial}{\partial s}s'(t). \tag{5.14}$$

The equation for the flux (3.8) at leading order in η is then

$$J = -h^3\Pi_z', \quad (h^3\Pi_z')_z = -r'(t)h_z \tag{5.15}$$

where $\Pi' = \Pi/\eta$. Noting that $r'(t) = -\Gamma_t \equiv$ the normal velocity of Γ, the solution to (5.15) is therefore

$$J = -\Gamma_t h, \tag{5.16}$$

where a no-flux boundary condition at $z = 0$ was used.

The contribution of the integral in (5.9) near the contact line can now be separated out. We shall find that it is formally of magnitude $\mathcal{O}(\ln \epsilon^{-1})$, compared to dissipation in the interior of the drop which is $\mathcal{O}(1)$ with respect to ϵ. Therefore, at leading order, only the former needs to be evaluated. Using $\theta(s) = h_r(0, s)$, expanding in r gives

$$h = rh_r(0, s) + \mathcal{O}(r^2) = \eta\theta z + \mathcal{O}(z^2\eta^2) \tag{5.17}$$

valid near the contact line.

The contribution to the dissipation integral near the contact line can be estimated on a strip $z_\epsilon < z < L$, where $h(z_\epsilon) = \epsilon$ and L is some "mesoscopic" cutoff such that $\epsilon \ll L \ll 1$. Using (5.17),

$$z_\epsilon = \frac{\epsilon}{\eta\theta} + \mathcal{O}(\epsilon^2/\eta). \tag{5.18}$$

Then by (5.16), (5.17) it follows that

$$\begin{aligned} D = \int_\Gamma \int_{z_\epsilon}^L \frac{\Gamma_t^2}{h}\,\eta^{-1}\,dz\,ds + \mathcal{O}(1) &= \int_\Gamma \int_{z_\epsilon}^L \frac{\Gamma_t^2}{\eta\theta z + \mathcal{O}(z^2\eta^2)}\,\eta^{-1}\,dz\,ds + \mathcal{O}(1) \\ &= \ln \epsilon^{-1} \int_\Gamma \frac{\Gamma_t^2}{\theta}\,ds + \mathcal{O}(1). \end{aligned} \tag{5.19}$$

Treating D as a bilinear form, it can be decomposed,

$$D(\Gamma_t, \delta\Gamma) = \ln \epsilon^{-1} \int_\Gamma \frac{\Gamma_t \, \delta\Gamma}{\theta} \, ds + B(\Gamma_t, \delta\Gamma), \tag{5.20}$$

where B is also bilinear since it is just the difference of D and the leading-order term. We can associate with B a linear operator $\mathscr{B}$, bounded independently of ϵ, so that

$$B(\Gamma_t, \delta\Gamma) = \int_\Gamma \delta\Gamma \, \mathscr{B}\Gamma_t \, ds. \tag{5.21}$$

Equating $D(\Gamma_t, \delta\Gamma)$ with (5.13), we have

$$\int_\Gamma \left(\ln \epsilon^{-1} \frac{\Gamma_t}{\theta} + \mathscr{B}\Gamma_t - \left[\theta_e^2/2 - \theta^2/2\right] \right) \delta\Gamma \, ds. \tag{5.22}$$

Since $\delta\Gamma$ is arbitrary, this means that the parenthetical term is zero. We can solve for Γ_t and restore physical scales, which gives the formula

$$\Gamma_t = \frac{\gamma}{6\mu} \left(\frac{\ln(H/\epsilon)}{\theta} \mathscr{I} + \mathscr{B} \right)^{-1} \left(\theta^2 - \theta_e^2\right) = \frac{\gamma}{6\mu \ln(H/\epsilon)} \theta \left(\theta^2 - \theta_e^2\right) + \mathcal{O}([\ln \epsilon^{-1}]^{-2}). \tag{5.23}$$

where $\mathscr{I}$ is the identity operator.

Several remarks about (5.23) are in order. The leading-order part of (5.23) was first proposed by deGennes [25] by means of a strictly local argument about energy and dissipation. The justification for this seems to rely heavily on the quasi-static assumption, which allowed the global energy change to be written only in terms of the contact line displacement (5.13). We also mention that the logarithmic dependence on ϵ was made rigorous in the estimates of Giacomelli & Otto [41].

The novel significance of (5.23) is that the correction term is only logarithmically smaller than the leading-order term in the small parameter ϵ. This correction term reflects the fact that the dissipation of energy in the droplet's interior can have a substantial effect on the motion. In general, this correction term is not easily computed. For the simple situations considered in section 6, however, one can make a full accounting of the energy dissipation.

Despite all this, at leading order we have derived a free boundary problem for Γ consisting of (5.10) and (5.23). Furthermore, the asymptotic calculation is self-consistent because the leading-order contact line velocity is slow (with respect to the parameter ϵ), and this justifies the quasi-static ansatz (5.6) in an *a posteriori* fashion.

6 Dynamical approximations

This section is devoted to consideration of simple flows in the context of the variational model. To make progress analytically, low-dimensional approximations are obtained by direct use of the method of section 2.3. It is particularly useful to examine how the overall flow geometry enters into the calculation of the dissipation expression, and to contrast this with the asymptotic results of § 5.

Comparisons will be made to the disjoining pressure model (4.3)–(4.4); some details of this computation were given in Glasner [43]. Initial conditions are specified that mimic

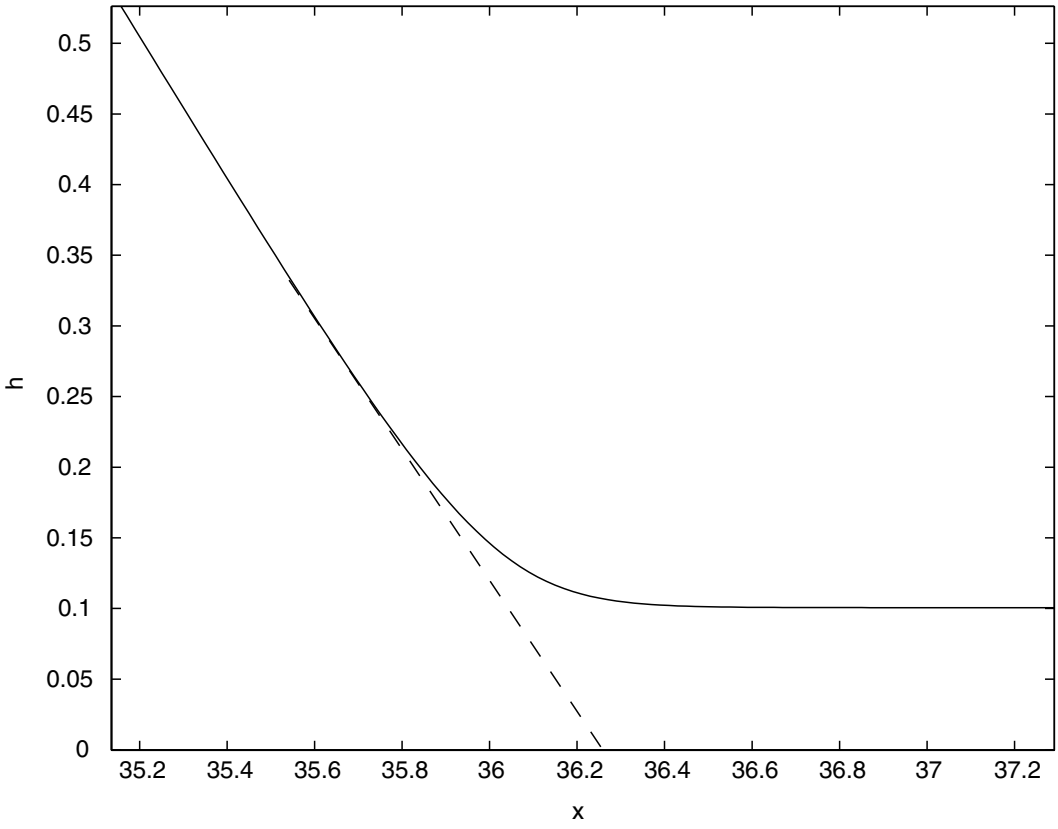

FIGURE 3. Equilibrium diffuse contact line region structure for the disjoining pressure model, where $\epsilon = 0.1$. The dashed line extrapolates the limiting contact line position.

the initial conditions for the Galerkin-type approximation, but where $h < \epsilon$, the PDE initial condition was replaced by $h = \epsilon$. The particular intermolecular potential employed here satisfies all the assumptions of §4:

$$U(h) = -1/2(\epsilon/h)^2 + 1/3(\epsilon/h)^3. \tag{6.1}$$

Other potentials which yield the same interfacial energies were also tried and gave virtually identical results. Since there is no true contact line in the PDE model, contact line positions were measured by linear extrapolation as in Figure 3.

6.1 Droplet spreading

We first consider the case where a sessile droplet spreads in response to capillary and gravitational forces (a pendant drop could be treated similarly). Gravity is included using the non-dimensional potential energy

$$\Phi(h) = \beta h^2/2, \quad \beta^2 = \frac{g\rho W^2}{\gamma_{LV}} = \text{Bond number}. \tag{6.2}$$

The approximation we will seek uses the quasi-static limit where droplet shapes are given by solving (5.10) where M is the integral of h over its support. The solution for

$\beta > 0$ is parametrized by the droplet's half-width W, and is

$$h(x;W) = \frac{M\beta/2}{\beta W - \tanh(\beta W)}\left[1 - \frac{\cosh\beta x}{\cosh\beta W}\right]. \tag{6.3}$$

The corresponding change in energy can be computed directly from (5.8) but is easier stated in terms of the contact angles using (5.13), which gives

$$dE = \left(\theta_e^2 - \theta^2\right)dW \tag{6.4}$$

where $\theta = \partial h/\partial x(W)$. The flux for a given change in W is found by direct solution of $J_x = -h_t = -\dot{W}\,\partial h/\partial w$ subject to zero boundary conditions, giving

$$J_s(x;W) = \dot{W}\frac{M\beta^2/2}{(\beta W\coth\beta W - 1)^2}\left[x - W\frac{\sinh\beta x}{\sinh\beta W}\right]. \tag{6.5}$$

The regularized dissipation integral is of the form

$$D(W) = \dot{W}^2\int_{-x_c}^{x_c}\frac{J_s^2(x;W)}{h^3(x;W)}\,dx, \quad h(x_c;W) = \epsilon. \tag{6.6}$$

In principle, the integral (6.6) can be evaluated analytically, but the result is too complicated to yield much insight. The author's earlier work [43], on the other hand, considered the situation with no gravity ($\beta = 0$), which proved to be more transparent. For completeness and clarity, we repeat some of the key steps from that paper.

In the case $\beta = 0$, the droplet shapes are parabolic

$$h = \frac{3M}{4W}\left(1 - \frac{x^2}{W^2}\right) \tag{6.7}$$

and the flux is the limit of (6.5) as $\beta \to 0$, which is

$$J = \frac{3M}{4W}\left(\frac{x}{W} - \frac{x^3}{W^3}\right)\dot{W}. \tag{6.8}$$

Letting $H = (3M)/(4W)$ be the height and $y = x/W$, the truncated dissipation integral can be written

$$\begin{aligned} D = \frac{W\dot{W}^2}{H}\int_{-\sqrt{1-\epsilon/H}}^{\sqrt{1-\epsilon/H}}\frac{(y-y^3)^2}{(1-y^2)^3}\,dy &= \frac{2W\dot{W}^2}{H}\ln\left(\frac{1+\sqrt{1-\epsilon/H}}{1-\sqrt{1-\epsilon/H}}\right) - 2\sqrt{1-\epsilon/H} \\ &= \frac{2W\dot{W}^2}{H}\left[\ln\epsilon^{-1} + \ln H + \ln 4 - 2 + \mathcal{O}(\epsilon)\right]. \end{aligned} \tag{6.9}$$

The role of energy dissipation in the bulk of the fluid is now obvious: it contributes a term $\ln H + \ln 4 - 2$ which is only logarithmically smaller than the leading-order term. Since the approximation is one-dimensional, (2.4) reduces simply to a balance of energy and its dissipation $dE/dt = -D$. We can obtain a formula for the contact-line velocity $\dot{W}$,

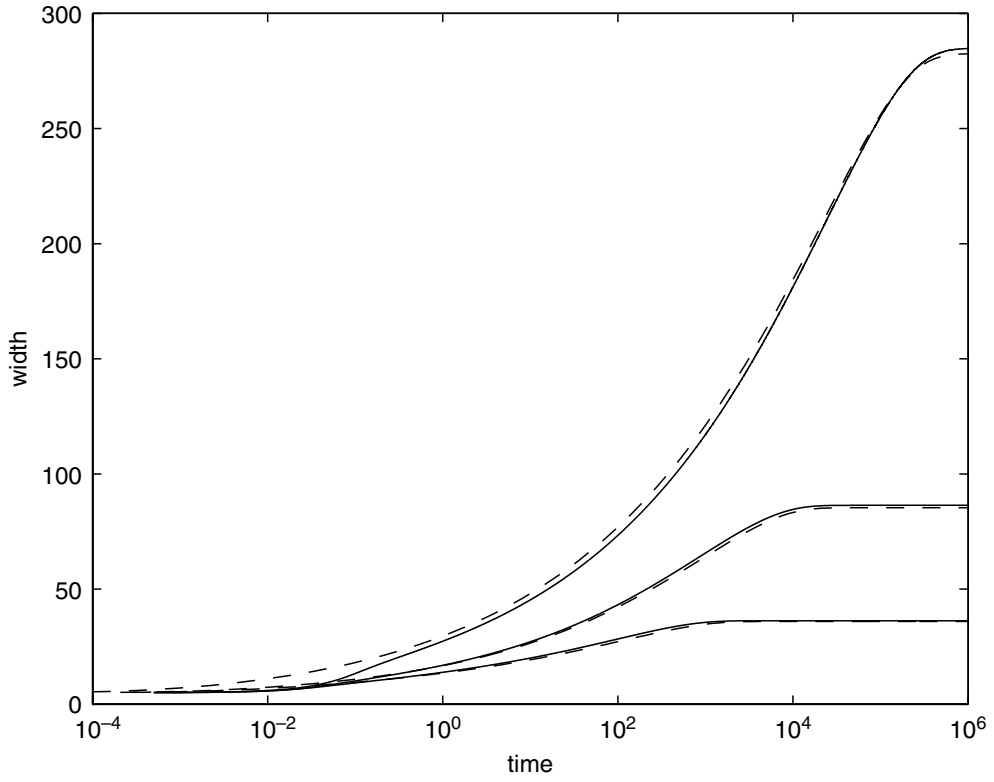

FIGURE 4. Width predicted by the disjoining pressure model (solid) versus the variational approximation (dotted). ¿From top to bottom, the values of β are $1, \sqrt{0.1}, 0.1$.

which in terms of the apparent contact angle is

$$\begin{aligned}\dot{W} &= \frac{\theta\left(\theta^2-\theta_e^2\right)}{\ln\epsilon^{-1}+\ln H+\ln 4-2+\mathcal{O}(\epsilon)}\\ &= \frac{\theta\left(\theta^2-\theta_e^2\right)}{\ln\epsilon^{-1}}(1-(\ln\epsilon^{-1})^{-1}(\ln H+\ln 4-2)+\mathcal{O}((\ln\epsilon^{-1})^{-2}))\end{aligned} \tag{6.10}$$

Note that the correction term is *not* local: it has a global dependence on the droplet height H. Obviously, any local (Tanner-like) contact line law could not account for this by itself. A similar calculation for axisymmetric drops gives a slightly different result [43], demonstrating that geometry as well as droplet height plays a role.

Returning to the general case $\beta \geqslant 0$ we can determine a single dynamical equation for W of the form

$$\dot{W} = -\frac{\theta_e^2-\theta^2}{D(W)}. \tag{6.11}$$

In practice, D is found numerically using efficient high-order adaptive quadrature. The results of solving both the ODE and PDE are presented in Figure 4. The model parameters were $\theta_e = \sqrt{1/3}$, $\epsilon = 0.1$, $M = 300$. There is considerable agreement between the lubrication dynamics and those of the variational model. A similar agreement was found for the case $\beta = 0$ in the previous work [43]. One may conclude that a sufficient accounting

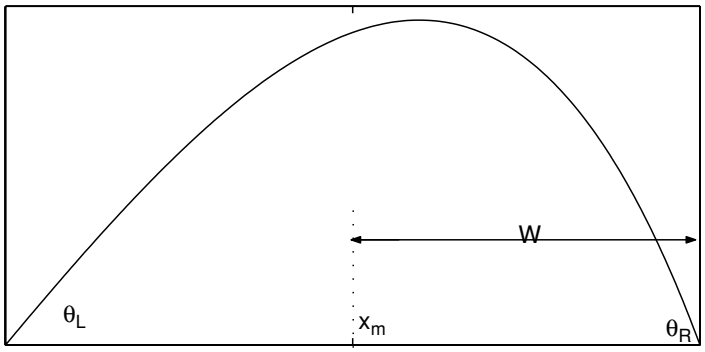

FIGURE 5. Quasi-steady sliding drop, parameterized by width W and center x_m.

of the energy dissipation has been made, and that the quasi-steady assumption is valid here. The main difference seems to be at early times in the PDE dynamics, where a transient solution results. This likely results from the initial data not being precisely on the inertial manifold, which the solution approaches at later times.

6.2 Sliding on an inclined surface

If the solid surface is inclined downward to the right at an angle α, the energy can be written

$$E = \int_\Omega \theta_e^2/2 + \frac{1}{2}|\nabla h|^2 + \beta \left[\frac{h^2}{2} - \tan(\alpha) h x\right] dx, \tag{6.12}$$

where the non-dimensional Bond number is now $\beta^2 = g\rho\cos(\alpha)W^2/\gamma_{LV}$. Quasi-steady solutions of (5.10) can be parameterized by two variables (Figure 5), the droplet midpoint x_m and the half-width W, giving

$$\begin{aligned} h(x; x_m, W) = {} & \frac{M\beta/2}{\beta W - \tanh(\beta W)} \left[1 - \frac{\cosh \beta y}{\cosh \beta W}\right] \\ & + \tan(\alpha) \left[y - W \frac{\sinh(\beta y)}{\sinh(\beta W)}\right], \quad y = x - x_m. \end{aligned} \tag{6.13}$$

As in (6.4), the change in energy can be related to the contact angles using (5.13). If x_R, θ_R and x_L, θ_L are the contact-line positions and angles on the right and left sides respectively, the energy change is

$$dE = \frac{\theta_e^2}{2}(2dW) - \frac{\theta_R^2}{2} dx_R + \frac{\theta_L^2}{2} dx_L = \left[\theta_e^2 - \frac{1}{2}\left(\theta_R^2 + \theta_L^2\right)\right] dW - \frac{1}{2}\left(\theta_R^2 + \theta_L^2\right) dx_m \tag{6.14}$$

since $w = (x_R - x_L)/2$ and $x_m = (x_R + x_L)/2$.

The fluid flux satisfies

$$-J_x = h_t = \frac{\partial h}{\partial W}\dot{W} + \frac{\partial h}{\partial x_m}\dot{x}_m. \tag{6.15}$$

This equation can be integrated using zero boundary conditions at the drop edges, and

the flux can be written as the sum of two separate components due to spreading and sliding as

$$J = J_{spread}\dot{w} + J_{slide}\dot{x}_m. \tag{6.16}$$

The translational component is readily found as $J_{slide} = h(x; x_m, W)$, and

$$J_{spread} = \frac{M\beta^2[y - w\sinh(\beta x)/\sinh(\beta W)]}{2(\beta w\coth(\beta W) - 1)} + \tan(\alpha)[\beta W\coth(\beta W) - 1]\left(\frac{\cosh(\beta W) - \cosh(\beta x)}{\sinh(\beta W)}\right). \tag{6.17}$$

The approximation of the form (2.9) is

$$\begin{pmatrix} D_{ww} & D_{wx} \\ D_{wx} & D_{xx} \end{pmatrix}\begin{pmatrix} \dot{W} \\ \dot{x}_m \end{pmatrix} = -\begin{pmatrix} \partial E/\partial w \\ \partial E/\partial x \end{pmatrix}. \tag{6.18}$$

The matrix coefficients are computed as

$$D_{ww} = \int_{h\geqslant\epsilon}\frac{J_{spread}^2}{h^3}dx, \quad D_{wx} = \int_{h\geqslant\epsilon}\frac{J_{spread}J_{slide}}{h^3}dx, \quad D_{xx} = \int_{h\geqslant\epsilon}\frac{J_{slide}^2}{h^3}dx. \tag{6.19}$$

The dynamics in (6.18) describe the coupled interaction of sliding and spreading. An asymptotic state is reached when spreading stops, and the drop slides in a steady manner, retaining the same shape as it moves. The resulting steady-state velocity V_∞ and width W_∞ can be found from (6.18) by solving the coupled equations

$$D_{xx}(W_\infty)V_\infty = -\frac{\partial E}{\partial x_m}, \quad D_{xw}(W_\infty)V_\infty = -\frac{\partial E}{\partial W}. \tag{6.20}$$

As in the previous example, a comparison with the lubrication PDE dynamics is made, in this case by computing the steady-state velocities. Figure 6 shows these velocities for each model as a function of slant angle α, showing a striking discrepancy (circles vs. x's) between the two. The explanation for this difference is that the variational model does not account for energy dissipation in the same way that the PDE does. As noted in § 4, subtle changes of the boundary conditions for the flux can have profound consequences. In particular, the sliding component of the flux $J_{slide} = h$ does not satisfy the matching condition (4.8). On the other hand, the modified sliding flux

$$J'_{slide} = h - \epsilon \tag{6.21}$$

does satisfy (4.8). The calculation was repeated with J'_{slide} in place of J_{slide}, and the steady-state velocity is in better agreement with that calculated from the PDE (circles vs. squares in Figure 6). As α increases however, the quasi-static assumption becomes less valid, reflected in the divergence between the predicted velocities in the PDE and variational approximations.

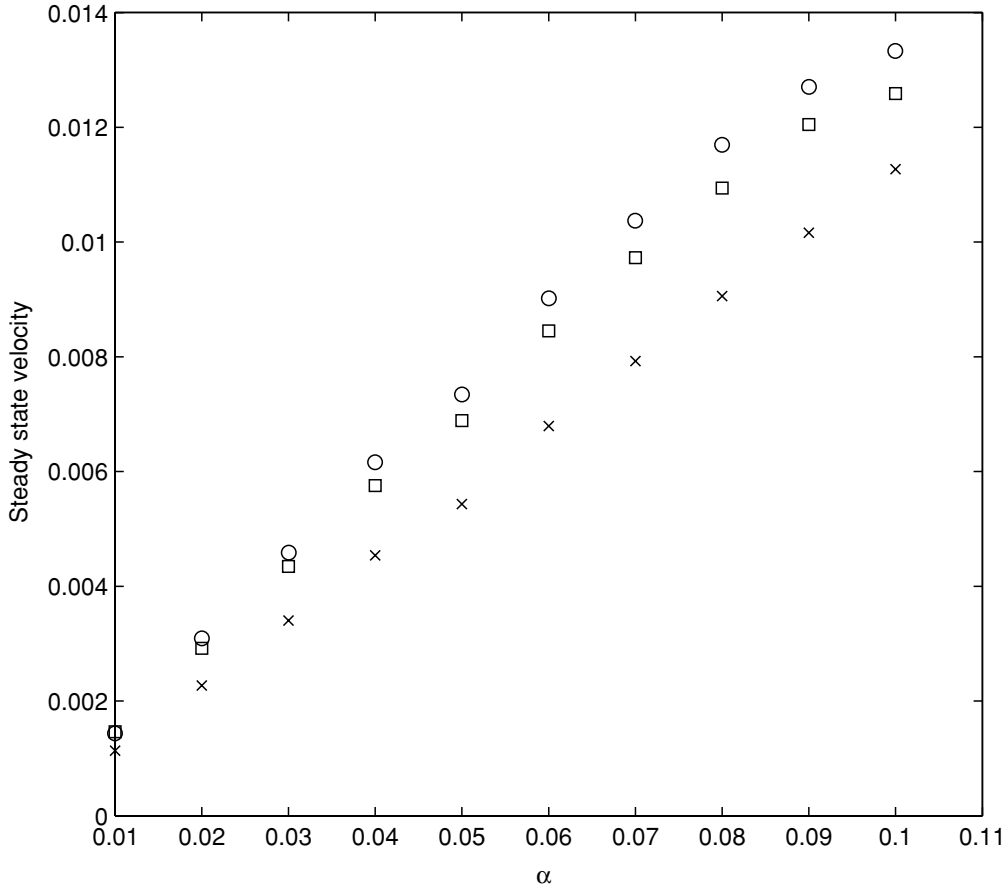

FIGURE 6. Steady-state velocities predicted by the disjoining pressure model (circles); the original variational approximation (x's); and the modification (squares) introduced by (6.21). Note that as the inclination angle increases, the quasi-static approximation becomes poor.

6.3 Droplet dewetting

In principle, (6.11) applies equally to quasi-static droplets which spread *or* contract toward equilibrium. The problem is that wide, shallow contracting drops can potentially violate the condition derived in section 5.2 that the aspect ratio is large in contrast to the capillary number.

Corrections to the assumed droplet shape can be obtained by iterative refinement, resulting in additional of degrees of freedom in the approximation. We will concentrate on the case where there is no gravity, and the leading order quasi-steady approximation (the $\beta = 0$ limit of (6.3)) is parameterized by the width W

$$h_0(x) = A\left(1 - \frac{x^2}{W^2}\right). \tag{6.22}$$

Rather than determining A from the constraint that the droplet have a given mass, we will find a correction to the shape and then invoke the constraint. The flux which results

from changes in W arises as before by solving $-J_x = h_t = (dh/dW)\dot{W}$, and has the form

$$J_0 \propto x\left(1 - \frac{x^2}{W^2}\right). \tag{6.23}$$

In the droplet interior the equation

$$J = -h^3 h_{xxx} \tag{6.24}$$

determines the exact flux. A shape correction arises from the fact that the leading-order flux (6.23) implies a non-constant value of h_{xxx}. More precisely, a correction of the form $h = h_0 + h_1$, where h_1 is small, can be inserted into (6.24) to give

$$\frac{J_0}{h_0^3} = (h_1)_{xxx}. \tag{6.25}$$

Integrating this expression and using the boundary conditions $h_1(\pm W) = 0$ gives the particular solution

$$h_1 \propto (1+y)\ln(1+y) + (1-y)\ln(1-y) - 2\ln 2, \quad y = x/W. \tag{6.26}$$

The true droplet shape is therefore better approximated by the linear combination

$$h = Ah_0(x;W) + Bh_1(x;W). \tag{6.27}$$

Now the mass constraint can be used, which implies a relationship between A, B and W. Writing the solution only terms of two of these variables, a two-parameter ansatz for the Galerkin procedure is obtained:

$$\begin{aligned} h(x;A,W) = {} & A(1-y^2) \\ & + \left(\frac{2A}{3} - \frac{M}{2W}\right)\left[\ln(1+y) + (1-y)\ln(1-y) - 2\ln 2\right], \quad y = x/W. \end{aligned} \tag{6.28}$$

Note that this refinement procedure can, in principle, be repeated indefinitely. The shape correction h_1 implies a flux correction J_1, which could then give a further correction h_2 by using (6.24).

As in the previous example, the energy gradients and dissipation expression can be computed in a straightforward but tedious fashion. For purposes of numerical computation, it is sufficient to do this using finite differences and quadratures, rather than analytically. The result is a system like (6.18) in the dynamic variables A, W. W still plays the role of the droplet half-width, and the droplet height can be computed as $H = A - 2\ln 2(2A/3 - M/2W)$.

Numerical comparisons between the PDE and one and two-dimensional approximations were made (Figure 7). The one dimensional quasi-static approximation diverges substantially from the PDE solution, indicating that this assumption is not satisfied. The two-dimensional approximation is, on the other hand, much better at predicting the PDE dynamics.

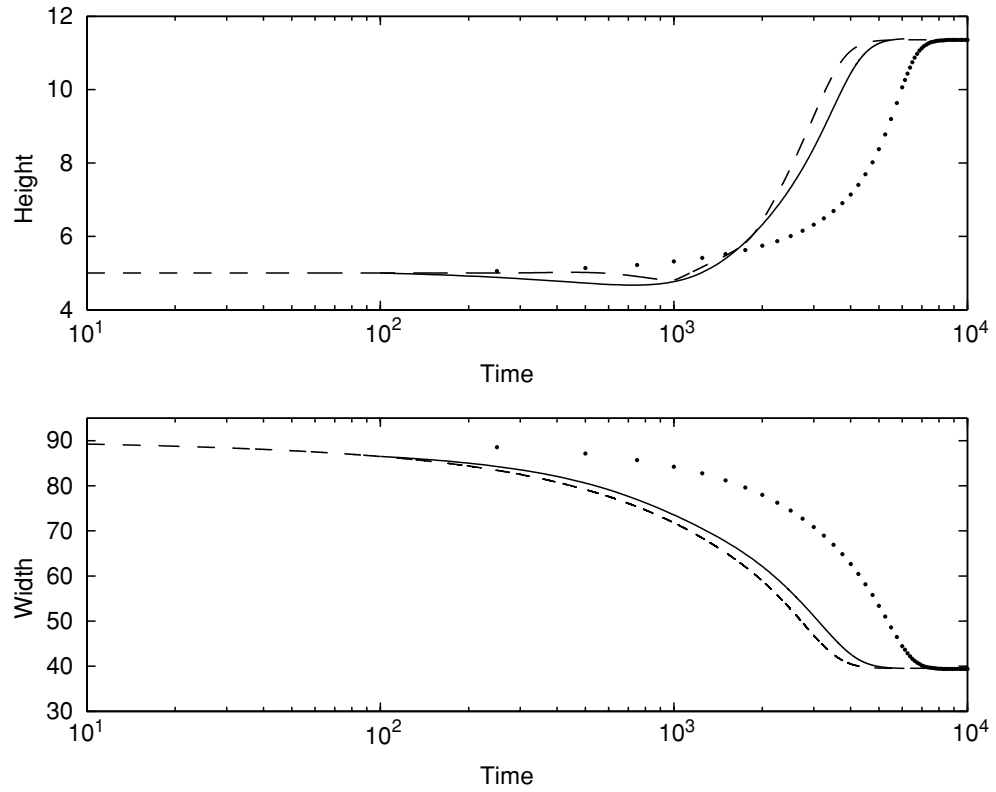

FIGURE 7. Symmetric contraction of a droplet. The height and width were measured for the PDE (dashed), and compared to the one-dimensional quasi-static approximation (dotted) and the two-dimensional approximation (solid) obtained from iterative refinement.

7 Conclusions

A different viewpoint to the dynamic contact line problem has been presented. No specific local structure or physics of the dynamic contact line was assumed, or even needed, in contrast to many other theories (e.g. [22, 39, 84, 93]). Provided that any microscopic mechanism for contact line motion can be characterized entirely by how energy is dissipated (which amounts to specifying ϵ), then the variational model may be useful as a universal framework in describing the *macroscopic* dynamics.

To a great extent, the present formulation is consistent with the equations of lubrication theory, although some subtle aspects of this relationship were noted. Because of this similarity, variationally constructed approximations as in § 6 could be alternatively regarded as analytic *methods*, as opposed to models in themselves. In addition, finite-dimensional reductions point the way to numerical algorithms which retain the variational structure.

The real strength of the variational approach may be best realized for dynamics which give rise to patterns and microstructure. Variational formulations can provide a definite mathematical notion of non-smooth solutions, for example, in magnetics [28] or crystallography [89]. Recent experimental evidence has shown that contact lines can have cusps and other fine-structure irregularities (see elsewhere [19, 82, 87]), which may be difficult to treat with traditional continuum models.

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