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Calculation of a key function in the asymptotic description of moving contact lines

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Abstract

An important element of the asymptotic description of flows having a moving liquid/gas interface which intersects a solid boundary is a function denoted $Q_i(\alpha)$ by Hocking and Rivers (1), where $0 < \alpha < \pi$ is the contact angle of the interface with the wall. $Q_i(\alpha)$ arises from matching of the inner and intermediate asymptotic regions introduced by those authors and is required in applications of the asymptotic theory. This article describes a new numerical method for the calculation of $Q_i(\alpha)$, which, because it explicitly allows for the logarithmic singularity in the kernel of the governing integral equation and uses quadratic interpolation of the nonsingular factor in the integrand, is more accurate than that employed by Hocking and Rivers. Nonetheless, our results show good agreement with theirs, with, however, noticeable departures near $\alpha = \pi$. We also discuss the limiting cases $\alpha \rightarrow 0$ and $\alpha \rightarrow \pi$. The leading-order terms of $Q_i(\alpha)$ in both limits are in accord with the analysis of Hocking (2). The next-order terms are also considered. Hocking did not go beyond leading order for $\alpha \rightarrow 0$ and we believe his results for the next order as $\alpha \rightarrow \pi$ to be incorrect. Numerically, we find that the next-order terms are $O(\alpha^2)$ for $\alpha \rightarrow 0$ and $O(1)$ as $\alpha \rightarrow \pi$. The latter result agrees with Hocking, but the value of the $O(1)$ constant does not. It is hoped that giving details of the numerical method and more precise information, both numerical and in terms of its limiting behaviour, concerning $Q_i(\alpha)$ will help those wanting to use the asymptotic theory of contact-line dynamics in future theoretical and numerical work.

1. Introduction

Flows with a moving fluid/fluid interface which intersects a solid wall are problematic because the usual model, i.e. the Navier-Stokes equations with a no-slip condition at the wall, leads to an unacceptable singularity at the contact line (see e.g. Moffatt (3), Huh and Scriven (4)). Although there is no agreed definitive model of this situation (Bonn *et al.* (5)), a commonly used one is to allow slip at the wall via a Navier condition in which slip is proportional to the shear rate, the constant of proportionality being referred to as the slip length and denoted λ .

In such a model, the slip length is very small, of the order of molecular scales, which leads to different matched asymptotic regions, the smallest of which being the inner region, for which the distance from the contact line is $O(\lambda)$. In addition to his notable later work on the lubrication approximation (see Hocking (6)), an analysis of the inner

region was given by Hocking (2) and forms the basis of the present paper. Subsequently, Hocking and Rivers (1) studied the slow spreading of a liquid droplet on a plane wall without gravity using matched asymptotic expansions. Their work is limited to the most commonly occurring case, in which the outer fluid is a gas of negligible viscosity (compared with the liquid), as is ours. Three asymptotic regions, namely inner, intermediate and outer, were used. The outer region represents the bulk of the drop, while, as its name suggests, the intermediate region corresponds to distances from the contact line which are small compared with the drop scale, but large compared with λ . Matching was applied between the outer and intermediate regions and between the intermediate and inner ones. The latter matching condition is expressed by equation (4.7) of Hocking and Rivers and involves information from the inner solution via a single function of the contact angle, α , denoted $j(\alpha)$. $j(\alpha)$ is in turn related to the function $Q_i(\alpha)$ (i for inner), which is the subject of this article, by their equation (5.10). This function is at the heart of the asymptotic theory and is required for its use.

Hocking and Rivers made a number of simplifying assumptions: axisymmetry, small Reynolds and Bond numbers and neglect of the unsteady term in the momentum equation. Because $Q_i(\alpha)$ arises from consideration of the flow at distances from the contact line which are much smaller than the drop size, the resulting inner/intermediate matching condition has more general applicability. For instance, there may be significant effects of fluid inertia and gravity in the outer region, but provided they do not reach down into the inner region, matching between the inner and intermediate regions is unaffected. Furthermore, we expect the flow near the contact line to be two dimensional so local application of the matching condition should be valid for asymmetric drops (see Cox (7)).

Interest in the function $Q_i(\alpha)$ has recently re-emerged in attempts to use the asymptotic theory to undertake numerical simulations of (possibly three-dimensional) flows with moving contact lines for realistic values of the slip length (Sui and Spelt (8), Sui, Ding and Spelt (9)). The computational costs of numerical simulations of the full problem (wherein the flow is resolved numerically down to the slip length) are prohibitive due to the very large range of length scales involved, but coupling the numerically resolved interface with the asymptotic theory to represent the unresolved flow has been demonstrated to yield useful results (Sui and Spelt (10), Solomenko, Spelt and Alix (11)).

This paper describes a new numerical method for calculating $Q_i(\alpha)$ and presents some results. The motivation is that only a table of values is given by Hocking and Rivers and details of the numerical method are not given, except to say it is based on that of Hocking (2). Referring to the latter paper, the method approximates the integral in equation [I.3.6] (where, here and henceforth, we refer to equation (x.y) of Hocking (2) as [I.x.y]) using the midpoint rule. Given the presence of a logarithmic singularity in the derivative of the integrand, one may ask questions about the numerical accuracy of

the results, questions which are not addressed by these authors. For these reasons, we revisit the numerical solution of the integral equation [I.3.1], providing a new method which allows for the singularity and is also more precise because it uses quadratic interpolation of the nonsingular part of the integrand. We believe it to be considerably more accurate.

The paper is organised as follows. Section 2 gives the integral equation which is subsequently solved numerically and the expression for $Q_i(\alpha)$ in terms of the solution. Section 3 concerns the leading-order behaviour of $Q_i(\alpha)$ in the limits $\alpha \rightarrow 0$ and $\alpha \rightarrow \pi$. Although these limits are addressed in Hocking (2), we give a brief description to prepare the reader for later numerical results. This is especially needed in the analysis of the $\alpha \rightarrow \pi$ limit, whose presentation by Hocking using Bessel functions of small order is best described as opaque and with which we disagree at higher order. Section 4 describes the numerical method, while section 5 gives results, compares them with those of Hocking and Rivers and examines their consequences in the limits $\alpha \rightarrow 0$ and $\alpha \rightarrow \pi$.

2. Formulation of the problem

The tangential stress at the wall in the liquid is given by the first of equations [I.2.18], where the nondimensional quantity $k(\rho)$ is governed by the integral equation [I.3.1], i.e.

$$1 - e^{-\rho} k(\rho) = \int_{-\infty}^{\infty} L(\rho - \rho') k(\rho') d\rho', \quad (2.1)$$

$\rho = \ln(r/\lambda)$, r is distance from the contact line and

$$L(\rho) = \frac{\pi}{4\alpha^2} \int_{|\rho|}^{\infty} \frac{\sinh \rho'}{\cosh \frac{\pi \rho'}{\alpha} - 1} d\rho', \quad (2.2)$$

which follows from [I.3.3] when $\rho > 0$. $L(\rho)$ is an even, positive function having a logarithmic singularity at $\rho = 0$ and which decays exponentially as $|\rho| \rightarrow \infty$. According to [I.3.5],

$$\int_{-\infty}^{\infty} L(\rho) d\rho = \frac{\alpha - \sin \alpha \cos \alpha}{2 \sin^2 \alpha} = \frac{1}{k_{\infty}}, \quad (2.3)$$

where k_{∞} is the $\rho \rightarrow +\infty$ limit of $k(\rho)$. In the opposite limit, $k(\rho) \rightarrow 0$ as $\rho \rightarrow -\infty$. Both limits are approached exponentially rapidly. Note that, to simplify the notation, we have dropped the subscript 1 from k and L .

Defining

$$\Gamma(\rho) = k(\rho) - k_\infty \quad \rho > 0, \quad (2.4)$$

$$\Gamma(\rho) = k(\rho) \quad \rho < 0, \quad (2.5)$$

$\Gamma(\rho)$ goes to zero as $\rho \rightarrow \pm\infty$. Using (2.3), (2.1) implies

$$e^{-\rho}\Gamma(\rho) + \int_{-\infty}^{\infty} L(\rho - \rho')\Gamma(\rho')d\rho' = k_\infty(K_0(\rho) - e^{-\rho}) \quad \rho > 0, \quad (2.6)$$

$$e^{-\rho}\Gamma(\rho) + \int_{-\infty}^{\infty} L(\rho - \rho')\Gamma(\rho')d\rho' = k_\infty K_0(\rho) \quad \rho < 0, \quad (2.7)$$

where

$$K_0(\rho) = \int_{\rho}^{\infty} L(\rho')d\rho'. \quad (2.8)$$

(2.6) and (2.7) provide an alternative form of the integral equation which will be used in the subsequent numerical method.

As $\rho \rightarrow +\infty$,

$$\int_{-\infty}^{\rho} k(\rho')d\rho' \sim k_\infty\rho + j(\alpha), \quad (2.9)$$

which defines the function $j(\alpha)$. Note that the corresponding equation, (4.6), of Hocking and Rivers is incorrect: there should be an integral over ρ on the left-hand side, as in our equation (2.9). Using (2.4) and (2.5),

$$j(\alpha) = \int_{-\infty}^{\infty} \Gamma(\rho)d\rho. \quad (2.10)$$

Equation (5.10) of Hocking and Rivers gives

$$Q_i(\alpha) = k_\infty^{-1} \int_{-\infty}^{\infty} \Gamma(\rho)d\rho \quad (2.11)$$

for the function which it is our aim to calculate. This requires determination of $\Gamma(\rho)$ and evaluation of the integral in (2.11).

3. The limits $\alpha \rightarrow 0$ and $\alpha \rightarrow \pi$ at leading order

3.1 Small α

When α is small, (2.2) implies that $L(\rho)$ is only significantly nonzero for $\rho = O(\alpha)$. Presuming variations of $k(\rho')$ take place over ranges of $O(1)$, as found numerically, $k(\rho')$ is approximated by $k(\rho)$ in (2.1). Using (2.3), this leads to

$$k(\rho) \sim \frac{1}{e^{-\rho} + k_{\infty}^{-1}}, \quad (3.1)$$

which corresponds to [I.3.17]. According to (3.1), $k(\rho)$ undergoes a transition from e^{ρ} behaviour to the constant value k_{∞} as ρ increases. The transition region is located at $\rho = \ln k_{\infty}$ and has $O(1)$ width. The latter of these results indicates that $k(\rho)$ does indeed vary over ranges of $O(1)$. The former result, combined with $k_{\infty} \sim 3\alpha^{-1}$ from (2.3), locates the transition region at $\rho = \ln(3\alpha^{-1})$. Thus, the transition region moves to increasingly large ρ as α decreases. This can be understood as follows. $\rho = \ln k_{\infty} + O(1)$ for the transition region corresponds to $r = O(k_{\infty}\lambda) = O(\alpha^{-1}\lambda)$, which means that the distance of the liquid/gas interface from the wall is $O(\lambda)$. Outside this region, slip at the wall is small, whereas inside it is significant. Thus, for small α , the condition for significant slip is that the distance of the interface from the wall be of the order of the slip length. As α decreases, significant slip occurs further and further from the contact line.

Using (2.4), (2.5) and (3.1),

$$\Gamma(\rho) \sim -\frac{k_{\infty}e^{-\rho}}{e^{-\rho} + k_{\infty}^{-1}} \quad \rho > 0, \quad (3.2)$$

$$\Gamma(\rho) \sim \frac{1}{e^{-\rho} + k_{\infty}^{-1}} \quad \rho < 0, \quad (3.3)$$

whose integration yields

$$\int_{-\infty}^{\infty} \Gamma(\rho) d\rho \sim -k_{\infty} \ln k_{\infty}. \quad (3.4)$$

Employing (2.11),

$$Q_i(\alpha) \sim -\ln k_{\infty} \sim \ln\left(\frac{1}{3}\alpha\right), \quad (3.5)$$

which agrees with [I.3.18].

3.2 α near π

It is shown in Appendix A that

$$L(\rho) = \frac{1}{4\alpha} \sum_{n=1}^{\infty} \left(\frac{e^{|\rho|}}{n\pi - \alpha} - \frac{e^{-|\rho|}}{n\pi + \alpha} \right) n\pi e^{-n\pi|\rho|/\alpha}. \quad (3.6)$$

Consider the first of the bracketed terms in (3.6) when $n = 1$. This term dominates the others as $\alpha \rightarrow \pi$, hence

$$L(\rho) \sim \frac{\pi e^{(1-\pi/\alpha)|\rho|}}{4\alpha(\pi-\alpha)} \sim \frac{e^{-\beta|\rho|}}{4\pi\beta}, \quad (3.7)$$

where $\beta = 1 - \alpha/\pi$ is small. (2.8) and (3.7) imply

$$K_0(\rho) \sim \frac{e^{-\beta\rho}}{4\pi\beta^2} \quad \rho > 0, \quad (3.8)$$

$$K_0(\rho) \sim \frac{2 - e^{\beta\rho}}{4\pi\beta^2} \quad \rho < 0. \quad (3.9)$$

(3.7)-(3.9) indicate that $L(\rho)$ and $K_0(\rho)$ have slow variations as functions of ρ . It might be thought that $\Gamma(\rho)$, the solution of (2.6), (2.7), would inherit these slow variations. However, this is not what is found numerically. Instead, it appears that

$$\beta^{-1}\Gamma(\rho) \rightarrow \Gamma_0(\rho) \quad (3.10)$$

as $\beta \rightarrow 0$, where $\Gamma_0(\rho)$ does not depend on β .

Consider (2.6) and (2.7) with $\rho, \rho' = O(1)$. (3.7)-(3.10), $k_\infty \sim 2\pi\beta^2$ (from (2.3)) and small β imply

$$\int_{-\infty}^{\infty} \Gamma_0(\rho) d\rho = 2\pi \quad (3.11)$$

at leading order. Thus, (2.11), $k_\infty \sim 2\pi\beta^2$ and (3.10) give

$$Q_i(\alpha) \sim \beta^{-1} = \frac{\pi}{\pi - \alpha}, \quad (3.12)$$

which is in agreement with the leading-order term of [I.3.29], though, as discussed later, we have doubts concerning the next-order term in that expansion. Note that, according to (3.5) and (3.12), $Q_i(\alpha)$ goes from $-\infty$ to $+\infty$ as α increases from 0 to π .

4. Numerical method

As noted earlier, calculation of $Q_i(\alpha)$ requires the solution of (2.6), (2.7) and the evaluation of the integral in (2.11). Both involve numerical approximations of integrals by sums. To this end, ρ is discretised and truncated to a finite range by defining

$$\rho_n = n\Delta \quad |n| \leq 2N, \quad (4.1)$$

where Δ is small and $\rho_{\max} = 2N\Delta$ is large. The unknown function $\Gamma(\rho)$ is represented by its values

$$\Gamma_n = \Gamma(\rho_n). \quad (4.2)$$

Because, given its definition by (2.4) and (2.5), $\Gamma(\rho)$ has a discontinuous jump at $\rho = 0$, there is a choice in the value to be given to Γ_0 . We define it as the limit of $\Gamma(\rho)$ as $\rho \rightarrow 0$ from below, the limit from above being $\Gamma_0 - k_\infty$. Within each interval $\rho_{2m} \leq \rho \leq \rho_{2m+2}$, $-N \leq m < N$, quadratic interpolation gives

$$\Gamma(\rho) = \Gamma_{2m+1} + \frac{\Gamma_{2m+2} - \Gamma_{2m}^*}{2\Delta} (\rho - \rho_{2m+1}) + \frac{\Gamma_{2m+2} + \Gamma_{2m}^* - 2\Gamma_{2m+1}}{2\Delta^2} (\rho - \rho_{2m+1})^2, \quad (4.3)$$

where $\Gamma_n^* = \Gamma_n$ for $n \neq 0$ and $\Gamma_0^* = \Gamma_0 - k_\infty$. Note that we do not use interpolation of the entire integrand in (2.6) and (2.7), just $\Gamma(\rho)$. This is because, as noted earlier, $L(\rho)$ has a logarithmic singularity, so doing so would degrade precision.

Equation (2.6) is applied with $\rho = \rho_n$, $0 < n \leq 2N$, and (2.7) is used for $\rho = \rho_n$, $-2N \leq n \leq 0$. The contribution of the interval $\rho_{2m} \leq \rho \leq \rho_{2m+2}$ to the integral in (2.6) and (2.7) is approximated using (4.3). Thus,

$$\begin{aligned} & \int_{\rho_{2m}}^{\rho_{2m+2}} L(\rho_n - \rho') \Gamma(\rho') d\rho' \\ &= \Gamma_{2m+1} d_{2m-n}^{(0)} + \left(\Gamma_{2m+2} - \Gamma_{2m}^* \right) \left(d_{2m-n}^{(1)} + \frac{1}{2} (n - 2m - 1) d_{2m-n}^{(0)} \right) \\ &+ \left(\Gamma_{2m+2} + \Gamma_{2m}^* - 2\Gamma_{2m+1} \right) \left(d_{2m-n}^{(2)} + 2(n - 2m - 1) d_{2m-n}^{(1)} + \frac{1}{2} (n - 2m - 1)^2 d_{2m-n}^{(0)} \right) \end{aligned} \quad (4.4)$$

where we have used the fact that $L(\rho)$ is an even function and introduced the notation

$$d_k^{(0)} = K_0(\rho_k) - K_0(\rho_{k+2}), \quad (4.5)$$

$$d_k^{(1)} = \frac{K_1(\rho_k) - K_1(\rho_{k+2})}{2\Delta}, \quad (4.6)$$

$$d_k^{(2)} = \frac{K_2(\rho_k) - K_2(\rho_{k+2})}{2\Delta^2}, \quad (4.7)$$

$$K_1(\rho) = \int_\rho^\infty \rho' L(\rho') d\rho', \quad K_2(\rho) = \int_\rho^\infty \rho'^2 L(\rho') d\rho'. \quad (4.8)$$

Summing over intervals and recalling the definition of Γ_n^* ,

$$\int_{-\rho_{\max}}^{\rho_{\max}} L(\rho_n - \rho') \Gamma(\rho') d\rho' = -k_{\infty} \left(d_{-n}^{(2)} + (2n-3)d_{-n}^{(1)} + \frac{1}{2}(n-1)(n-2)d_{-n}^{(0)} \right) + e_n \Gamma_{2N} + f_n \Gamma_{-2N} - \sum_{m=-N}^{N-1} b_{2m-n} \Gamma_{2m+1} + \sum_{m=1-N}^{N-1} c_{2m-n} \Gamma_{2m}, \quad (4.9)$$

where

$$b_k = 2d_k^{(2)} - 4(k+1)d_k^{(1)} + \left((k+1)^2 - 1 \right) d_k^{(0)}, \quad (4.10)$$

$$c_k = d_k^{(2)} + d_{k-2}^{(2)} - (2k+3)d_k^{(1)} - (2k-3)d_{k-2}^{(1)} + \frac{1}{2} \left((k+1)(k+2)d_k^{(0)} + (k-1)(k-2)d_{k-2}^{(0)} \right). \quad (4.11)$$

$$e_n = d_{2N-n-2}^{(2)} + (2n-4N+3)d_{2N-n-2}^{(1)} + \frac{1}{2}(n-2N+1)(n-2N+2)d_{2N-n-2}^{(0)}, \quad (4.12)$$

$$f_n = d_{-2N-n}^{(2)} + (2n+4N-3)d_{-2N-n}^{(1)} + \frac{1}{2}(n+2N-1)(n+2N-2)d_{-2N-n}^{(0)}. \quad (4.13)$$

Neglecting the contribution from $|\rho'| > \rho_{\max}$, because $\Gamma(\rho')$ is exponentially small at large $|\rho'|$, (4.9) is a numerical approximation of the integral in (2.6) and (2.7) when $\rho = \rho_n$. The result is a system of $4N+1$ linear equations for the unknowns Γ_n . This system is solved using LAPACK routine DGESV. Appendix B describes the numerical calculation of the functions $K_0(\rho)$, $K_1(\rho)$ and $K_2(\rho)$.

As for the integrals in (2.6) and (2.7), the contribution to the integral in (2.11) from $|\rho| > \rho_{\max}$ is neglected on the grounds that $\Gamma(\rho)$ is exponentially small at large $|\rho|$. The contribution from $|\rho| \leq \rho_{\max}$ is approximated using (4.3), leading to

$$\int_{-\rho_{\max}}^{\rho_{\max}} \Gamma(\rho) d\rho = \frac{2}{3} \Delta \left(\sum_{m=1-N}^{N-1} (\Gamma_{2m} + 2\Gamma_{2m+1}) + 2\Gamma_{1-2N} + \frac{1}{2}(\Gamma_{2N} + \Gamma_{-2N} - k_{\infty}) \right), \quad (4.14)$$

which amounts to Simpson's rule. Finally, (2.11) gives $Q_i(\alpha)$.

The above procedure should converge to the true value of $Q_i(\alpha)$ as the numerical parameters, Δ , N , and K (which is the number of terms in the truncated series (B.4)-(B.7)), approach the limits $\Delta \rightarrow 0$, $N\Delta \rightarrow \infty$ and $K \rightarrow \infty$. Thus, the numerical parameters were varied and convergence sought. The exact value $Q_i(\pi/2) = \gamma - \ln 2 = -0.1159315$ (γ is Euler's constant) follows from [I.3.10] and was used as a check. The numerical value using $\Delta = 0.1$, $N = 200$ and $K = 10$ agreed to the given seven decimal places of accuracy. For other values of α , comparisons between different choices of Δ , N , and K were made.

Concerning convergence with increasing K , for $K \geq 10$ and the large $N\Delta$ required for convergence, we found that it was limited by machine precision (IEEE double precision was used throughout). Thus, $K = 10$ was adopted. Varying Δ and N , it was found that the most important constraint is that of large $N\Delta$. We found that $\Delta = 0.1$, $N = 200$ and $K = 10$ lead to values of $Q_i(\alpha)$ with better than six decimal places of precision for the values of α in Table 1 and the following results use these numerical parameters.

5. Results

Results of both our calculations and those of Hocking and Rivers are given in Table 1. There is good agreement for lower values of α , but larger differences appear when α approaches π . For instance, compared to ours for $\alpha = 2.9$ and $\alpha = 3.0$, their values of Q_i differ from ours by $\sim 2\%$ and $\sim 8\%$. The results also disagree to a lesser extent for smaller α . For instance, when $\alpha = 0.5$, we find $Q_i = -1.751748$, compared with $Q_i = -1.7519$ from Hocking and Rivers. In any case, it is clear that the tabulated results of Hocking and Rivers should not be relied on to give the precision suggested by their table.

Fig. 1 shows $Q_i(\alpha)$ as a function of α . It is apparent that, as we found analytically in section 3, $Q_i(\alpha)$ goes from $-\infty$ to $+\infty$ as α increases from 0 to π , passing through zero when $\alpha = \alpha_0$, where $\alpha_0 = 1.642671$. The leading-order limiting forms, (3.5) as $\alpha \rightarrow 0$ and (3.12) as $\alpha \rightarrow \pi$, are well respected by the numerical results. Because the next-order terms are, by definition, small compared with the leading-order ones, accuracy of their numerical determination is a challenge. Nonetheless, thanks to the intrinsic precision of the present scheme, clear results emerge. Fig. 2 plots the difference between $Q_i(\alpha)$ and the logarithmic form, (3.5), divided by α^2 . It appears that the next term in the small- α expansion (3.5) is $O(\alpha^2)$, the numerically determined coefficient of that term being ≈ 0.156 .

| α | A | B | α | A | B |
|----------|-----------|---------|----------|-----------|---------|
| 0.1 | -3.399640 | -3.3982 | 1.6 | -0.069580 | -0.0696 |
| 0.2 | -2.701800 | -2.7011 | 1.7 | 0.097430 | 0.0974 |
| 0.3 | -2.288442 | -2.2880 | 1.8 | 0.280572 | 0.2805 |
| 0.4 | -1.989559 | -1.9905 | 1.9 | 0.485179 | 0.4850 |
| 0.5 | -1.751748 | -1.7519 | 2.0 | 0.718325 | 0.7181 |
| 0.6 | -1.551079 | -1.5509 | 2.1 | 0.989705 | 0.9888 |
| 0.7 | -1.374626 | -1.3745 | 2.2 | 1.313059 | 1.3112 |
| 0.8 | -1.214487 | -1.2143 | 2.3 | 1.708597 | 1.7053 |
| 0.9 | -1.065352 | -1.0653 | 2.4 | 2.207374 | 2.2010 |
| 1.0 | -0.923350 | -0.9231 | 2.5 | 2.859730 | 2.8487 |
| 1.1 | -0.785429 | -0.7853 | 2.6 | 3.753054 | 3.7349 |
| 1.2 | -0.648990 | -0.6489 | 2.7 | 5.053636 | 5.0312 |
| 1.3 | -0.511644 | -0.5116 | 2.8 | 7.121957 | 7.0840 |

| | | | | | |
|-----|-----------|---------|-----|-----------|---------|
| 1.4 | -0.371022 | -0.3710 | 2.9 | 10.914176 | 10.6700 |
| 1.5 | -0.224612 | -0.2246 | 3.0 | 20.084725 | 21.6400 |

TABLE 1. Values of $Q_i(\alpha)$ according to the present calculations (A) and Hocking and Rivers (B).

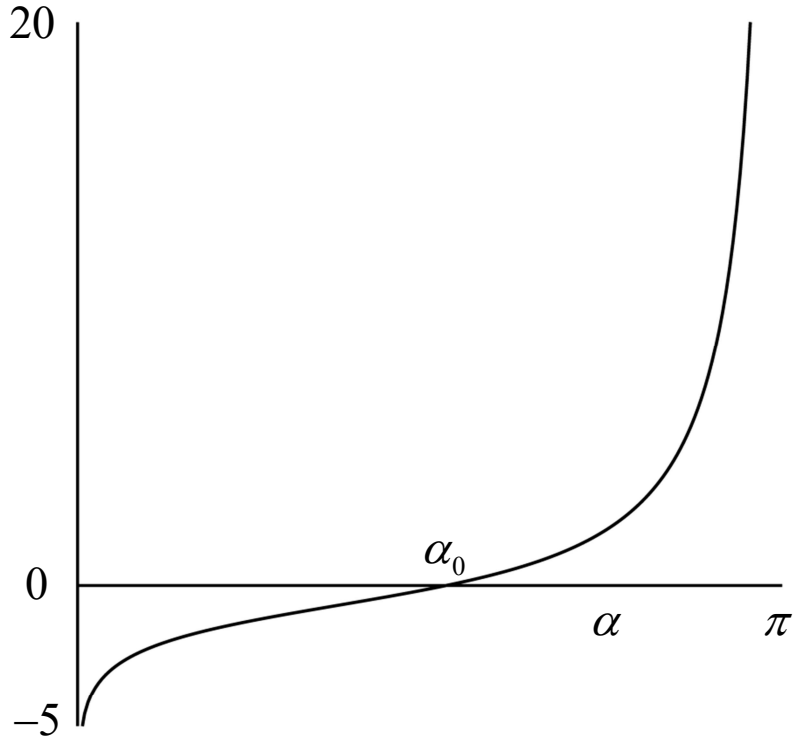


FIG. 1. Numerically determined $Q_i(\alpha)$.

Concerning the limit $\alpha \rightarrow \pi$, Fig. 3 shows the difference between $Q_i(\alpha)$ and the limiting form, (3.12), implying

$$Q_i \sim \frac{\pi}{\pi - \alpha} + C \quad (5.1)$$

as $\alpha \rightarrow \pi$. The first term in (5.1) corresponds to (3.12), whereas the second is a higher-order correction. Our numerical results indicate $C \approx -2.116$, which is clearly different from the value, $C = 2\gamma - \ln(2\pi) = -0.683446$, obtained from [I.3.29]. Given the opacity of the analysis leading to that equation, it is difficult to know the precise reasons for this higher-order discrepancy. However, it seems to us that even the first step in the analysis, namely the approximation of the integral equation by [I.3.21], although justified at leading order, is inadequate at the order considered here. Our numerical results suggest a value close to $C = \gamma - \ln 2 - 2 = -2.115932$ and, although being unable to prove it, we conjecture that this is the exact value.

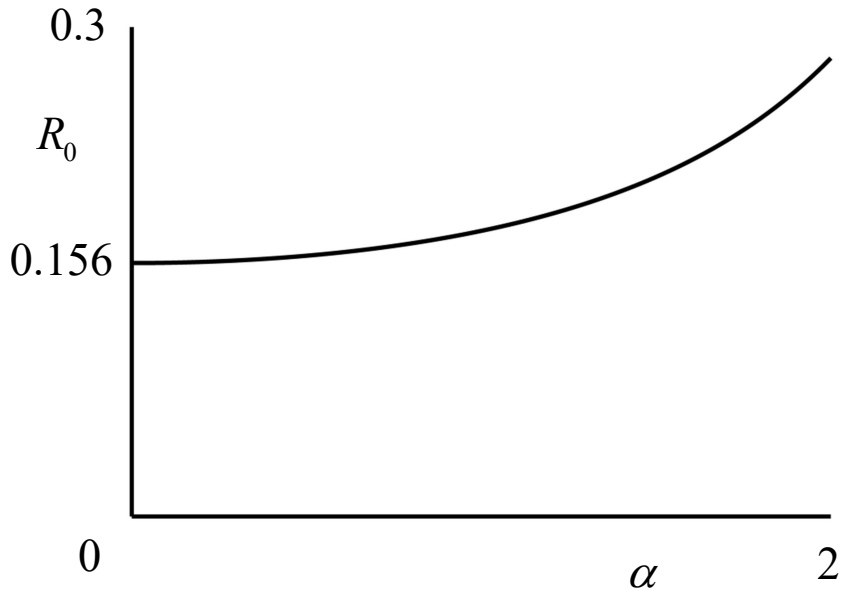


FIG. 2. $R_0 = \alpha^{-2} (Q_i(\alpha) - \ln(\alpha/3))$ as a function of α .

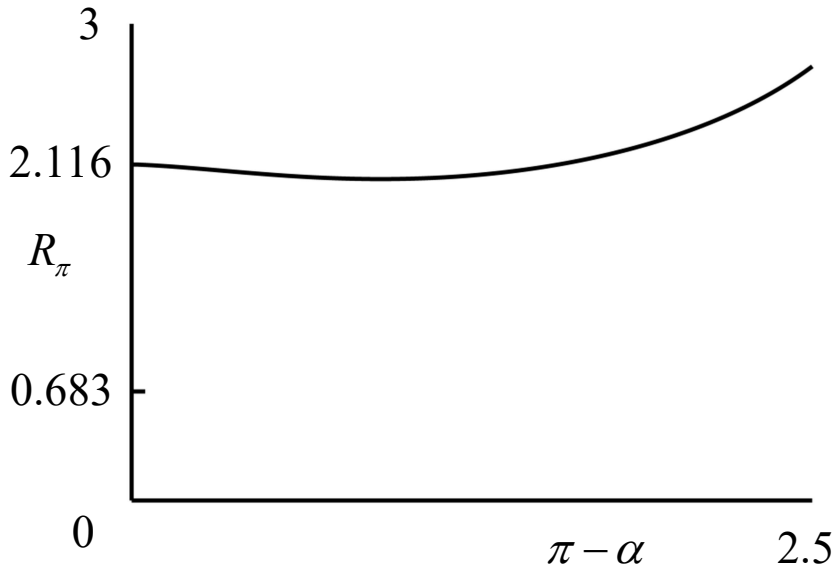


FIG. 3. $R_\pi = \pi / (\pi - \alpha) - Q_i(\alpha)$ as a function of $\pi - \alpha$. The $\alpha \rightarrow \pi$ limiting value, 0.683446, of Hocking (2) is also indicated.

6. Conclusions

The function $Q_i(\alpha)$, defined by Hocking and Rivers (1), plays a key role in the asymptotic theory of liquid/gas flows with moving contact lines on a wall. In this paper, we have described a new numerical method for its calculation, which we believe to be more accurate than its predecessors because, in dealing with the underlying integral equation, it takes

explicit account of a logarithmic singularity and uses a higher-order scheme for the nonsingular part of the integrand. We have given results obtained using this method and compared them with those of Hocking and Rivers (1). The agreement is good at smaller values of α , though not perfect, and less so as $\alpha = \pi$ is approached. The limits $\alpha \rightarrow 0$ and $\alpha \rightarrow \pi$ have also been examined. Our results agree with Hocking (2) at leading order, i.e. $Q_i(\alpha) \sim \ln(\alpha/3)$ as $\alpha \rightarrow 0$ and $Q_i(\alpha) \sim \pi/(\pi - \alpha)$ as $\alpha \rightarrow \pi$. However, Hocking did not go beyond leading order for $\alpha \rightarrow 0$ and we believe his result for the next order as $\alpha \rightarrow \pi$ to be incorrect. Our results indicate that the next order term in the small α expansion is $O(\alpha^2)$, the numerically determined coefficient of that term being ≈ 0.156 , while as $\alpha \rightarrow \pi$, the expansion proceeds as $Q_i(\alpha) \sim \pi/(\pi - \alpha) + C$, where $C \approx -2.116$, whereas Hocking claimed that $C = 2\gamma - \ln(2\pi) = -0.683446$, where γ is Euler's constant. Our numerical value of C is close to $\gamma - \ln 2 - 2 = -2.115932$ and, although being unable to prove it, we conjecture that this is the exact value.

We hope that the numerical scheme and results presented here will interest those, be they theorists or those inclined to numerical simulation, wanting to exploit matched asymptotic methods for the study of flows with moving contact lines.

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Appendix A: Demonstration of equation (3.6)

Let

$$\hat{L}(\rho) = \frac{1}{4\alpha} \sum_{n=1}^{\infty} \left(\frac{e^{\rho}}{n\pi - \alpha} - \frac{e^{-\rho}}{n\pi + \alpha} \right) n\pi e^{-n\pi\rho/\alpha} \quad (\text{A.1})$$

for $\rho > 0$. Differentiating (A.1),

$$\begin{aligned} \frac{d\hat{L}}{d\rho} &= -\frac{1}{4\alpha^2} (e^{\rho} - e^{-\rho}) \sum_{n=1}^{\infty} n\pi e^{-n\pi\rho/\alpha} \\ &= -\frac{1}{2\alpha^2} \sinh \rho \sum_{n=1}^{\infty} n\pi e^{-n\pi\rho/\alpha} \end{aligned} \quad (\text{A.2})$$

We have

$$\begin{aligned} \sum_{n=1}^{\infty} n\pi e^{-n\pi\rho/\alpha} &= -\alpha \frac{d}{d\rho} \sum_{n=0}^{\infty} e^{-n\pi\rho/\alpha} = -\alpha \frac{d}{d\rho} \frac{1}{1 - e^{-\pi\rho/\alpha}} \\ &= \frac{\pi e^{-\pi\rho/\alpha}}{(1 - e^{-\pi\rho/\alpha})^2} = \frac{\pi}{2 \left(\cosh \frac{\pi\rho}{\alpha} - 1 \right)} \end{aligned} \quad (\text{A.3})$$

Combining (A.2) and (A.3),

$$\frac{d\hat{L}}{d\rho} = -\frac{\pi}{4\alpha^2} \frac{\sinh \rho}{\cosh \frac{\pi\rho}{\alpha} - 1}. \quad (\text{A.4})$$

According to (A.1), $\hat{L}(\rho) \rightarrow 0$ as $\rho \rightarrow \infty$, hence the integral of (A.4) gives $\hat{L}(\rho) = L(\rho)$ for $\rho > 0$, where (2.2) has been used. Thus, (3.6) applies when $\rho > 0$. Because both the left- and right-hand sides of that equation are even functions of ρ , it also holds for $\rho < 0$.

Appendix B: Calculation of $K_0(\rho)$, $K_1(\rho)$ and $K_2(\rho)$

$K_0(\rho)$, $K_1(\rho)$ and $K_2(\rho)$ are given by (2.8), (4.8) and (4.9). The fact that $L(\rho)$ is an even function implies

$$K_0(-\rho) = 2K_0(0) - K_0(\rho), \quad (\text{B.1})$$

$$K_1(-\rho) = K_1(\rho). \quad (\text{B.2})$$

$$K_2(-\rho) = 2K_2(0) - K_2(\rho). \quad (\text{B.3})$$

Thus, we can restrict attention to $\rho \geq 0$. The values of $K_0(\rho)$, $K_1(\rho)$ and $K_2(\rho)$ are then required at $\rho = n\Delta$, $0 \leq n \leq 4N$.

Using (3.6) to determine $L(\rho)$, $K_0(\rho)$, $K_1(\rho)$ and $K_2(\rho)$ gives series which are rapidly convergent when ρ is large and positive. They are numerically calculated by truncation:

$$L(\rho) = \frac{1}{4\alpha} \sum_{n=1}^K \left(\frac{e^\rho}{n\pi - \alpha} - \frac{e^{-\rho}}{n\pi + \alpha} \right) n\pi e^{-n\pi\rho/\alpha}, \quad (\text{B.4})$$

$$K_0(\rho) = \frac{1}{4} \sum_{n=1}^K \left(\frac{e^\rho}{(n\pi - \alpha)^2} - \frac{e^{-\rho}}{(n\pi + \alpha)^2} \right) n\pi e^{-n\pi\rho/\alpha}, \quad (\text{B.5})$$

$$K_1(\rho) = \frac{1}{4} \sum_{n=1}^K \left(\frac{e^\rho}{(n\pi - \alpha)^2} \left(\rho + \frac{\alpha}{n\pi - \alpha} \right) - \frac{e^{-\rho}}{(n\pi + \alpha)^2} \left(\rho + \frac{\alpha}{n\pi + \alpha} \right) \right) n\pi e^{-n\pi\rho/\alpha}, \quad (\text{B.6})$$

$$K_2(\rho) = \frac{1}{4} \sum_{n=1}^K \left(\frac{e^\rho}{(n\pi - \alpha)^2} \left(\rho^2 + \frac{2\alpha}{n\pi - \alpha} \rho + 2 \left(\frac{\alpha}{n\pi - \alpha} \right)^2 \right) - \frac{e^{-\rho}}{(n\pi + \alpha)^2} \left(\rho^2 + \frac{2\alpha}{n\pi + \alpha} \rho + 2 \left(\frac{\alpha}{n\pi + \alpha} \right)^2 \right) \right) n\pi e^{-n\pi\rho/\alpha}. \quad (\text{B.7})$$

(B.4)-(B.7) provide $L(\rho)$, $K_0(\rho)$, $K_1(\rho)$ and $K_2(\rho)$ for $\rho = 4N\Delta$. However, convergence is slower when ρ is reduced and a different method is needed.

According to (2.2), (2.8), (4.8) and (4.9),

$$\frac{d\hat{L}}{d\rho} = \frac{1}{2\pi\rho} - \frac{\pi}{4\alpha^2} \frac{\sinh \rho}{\cosh \frac{\pi\rho}{\alpha} - 1}, \quad (\text{B.8})$$

$$\frac{d\hat{K}_0}{d\rho} = -\hat{L} - \frac{1}{2\pi}, \quad (\text{B.9})$$

$$\frac{d\hat{K}_1}{d\rho} = -\rho \left(\hat{L} + \frac{1}{4\pi} \right), \quad (\text{B.10})$$

$$\frac{d\hat{K}_2}{d\rho} = -\rho^2 \left(\hat{L} + \frac{1}{6\pi} \right), \quad (\text{B.11})$$

where

$$\hat{L} = L + \frac{1}{2\pi} \ln \rho, \quad (\text{B.12})$$

$$\hat{K}_0 = K_0 - \frac{1}{2\pi} \rho \ln \rho, \quad (\text{B.13})$$

$$\hat{K}_1 = K_1 - \frac{1}{4\pi} \rho^2 \ln \rho, \quad (\text{B.14})$$

$$\hat{K}_2 = K_2 - \frac{1}{6\pi} \rho^3 \ln \rho. \quad (\text{B.15})$$

The change of variables from L , K_0 , K_1 and K_2 to \hat{L} , \hat{K}_0 , \hat{K}_1 and \hat{K}_2 removes the singularity at $\rho = 0$. A fourth-order Runge-Kutta scheme with step δ is used to integrate (B.8)-(B.11) downwards in ρ , beginning at $\rho = 4N\Delta$ and values of \hat{L} , \hat{K}_0 , \hat{K}_1 and \hat{K}_2 from (B.12)-(B.15), with those of L , K_0 , K_1 and K_2 from (B.4)-(B.7). The step length is $\delta = \Delta/M$, where M is a positive integer. Thus, required values of K_0 , K_1 and K_2 are

obtained using (B.13)-(B.15) every M steps. To maintain precision at small α , M is chosen to be the smallest integer greater than α^{-1} .

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