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Boundary-value problems in the theory of lipid membranes

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Abstract General contact conditions are developed for lipid membranes interacting with curved substrates along their edges. These include the anchoring conditions familiar from liquid-crystal theory and accommodate non-uniform membranes and non-uniform adhesion between a bulk fluid or membrane and a rigid substrate. The theory is illustrated through explicit solutions and numerical simulations.

Keywords Lipid membranes · Bilayers · Anchoring conditions · Adhesion

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1 Introduction

Much of the literature on lipid membranes is concerned with membranes without boundary that are either closed or unbounded [1]. However, boundary conditions are central to the function of lipid membranes interacting with biological structures such as transmembrane proteins [2]. Recently some authors have advanced the theoretical underpinnings of the subject through careful consideration of the equilibrium conditions holding at the edge of a membrane interacting with a substrate [3,4]. In the present work we generalize these conditions to accommodate arbitrarily curved substrates, non-uniform membrane properties and non-uniform membrane–substrate interactions.

Section 2 briefly introduces the geometric setting and the basic variational problem from which the rest of the work proceeds. In Sect. 3 we present a concise account of the variational derivation of the Euler–Lagrange equations holding in the interior of the membrane. These include a simple condition restricting the surface tension in the case of non-uniform membrane properties as well as the associated generalization of the well-known *shape equation* [1,3,5,6]. Granted these, the conditions holding at an edge of the membrane are obtained from the residual stationary-energy principle in Sect. 4, which constitutes the main part of the paper. These include consideration of edge forces and couples as well as the adhesion between a bulk fluid exposed to a rigid wall and interacting with the membrane. Lipid membranes may be regarded as two-dimensional liquid crystals whose structure is conferred by the oriented lipid molecules. Accordingly we adapt the well-known *anchoring* conditions of liquid-crystal theory [7,8] to the case of membranes. Their role is illustrated analytically and numerically in the remainder of Sect. 4. The linearized theory, valid for small deviations of the membrane from a plane, is developed in Sect. 5, and explicit solutions to the associated equations are compared to numerical

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simulations based on the exact nonlinear theory. Finally, in Sect. 6 we outline the theory of adhesion for closed vesicles interacting with rigid substrates. The required adjustment to the basic theory is limited to a condition at the edge marking the transition from the free part of the membrane to the part in contact with the substrate. This restricts the jump in curvature at the transition and effectively furnishes a free-boundary condition. While this result is well-known in principle [3, 4], its derivation is given here under general conditions consistent with a local constraint on surface area, appropriate for potentially non-uniform membranes, in favor of the global constraint adopted universally in the literature. The condition is illustrated through numerical simulations of axisymmetric vesicles interacting with curved substrates under the action of point loads applied at their poles.

2 Surface geometry and the energy functional

The response of the membrane is embodied in an areal free-energy density $W(H, K; \theta^\alpha)$, where H is the mean curvature of the membrane surface ω and K is the Gaussian curvature. These are defined by

$$H = \frac{1}{2}a^{\alpha\beta}b_{\alpha\beta} \quad \text{and} \quad K = \frac{1}{2}\varepsilon^{\alpha\beta}\varepsilon^{\lambda\mu}b_{\alpha\lambda}b_{\beta\mu}, \quad (1)$$

where $(a^{\alpha\beta})$ is the matrix of dual metric components, the inverse of the metric $(a_{\alpha\beta})$; $\varepsilon^{\alpha\beta} = e^{\alpha\beta}/\sqrt{a}$ is the permutation tensor density with $a = \det(a_{\alpha\beta})$; $e^{12} = -e^{21} = 1$, $e^{11} = e^{22} = 0$; and $b_{\alpha\beta}$ are the coefficients of the second fundamental form. The latter are the covariant components of the surface curvature tensor. The contravariant *cofactor* of the curvature is given by

$$\tilde{b}^{\alpha\beta} = \varepsilon^{\alpha\lambda}\varepsilon^{\beta\gamma}b_{\lambda\gamma}, \quad (2)$$

and satisfies

$$b_\mu^\beta \tilde{b}^{\mu\alpha} = K a^{\beta\alpha}, \quad (3)$$

where b_μ^β are the mixed components of the curvature. These components figure in the Gauss and Weingarten equations

$$\mathbf{a}_{\alpha;\beta} = b_{\alpha\beta}\mathbf{n} \quad \text{and} \quad \mathbf{n}_{,\alpha} = -b_\alpha^\beta \mathbf{a}_\beta, \quad (4)$$

respectively. Here, $\mathbf{a}_\alpha = \mathbf{r}_{,\alpha}$ are the tangent vectors to ω induced by the parametrization $\mathbf{r}(\theta^\alpha)$, the position in 3-space of a point on the surface with coordinates θ^α , and the unit-vector field $\mathbf{n}(\theta^\alpha) = \frac{1}{2}\varepsilon^{\alpha\beta}\mathbf{a}_\alpha \times \mathbf{a}_\beta$ is the local surface orientation. The $\mathbf{a}_\alpha$ are related to the metric by $a_{\alpha\beta} = \mathbf{a}_\alpha \cdot \mathbf{a}_\beta$, where the dot refers to the conventional Euclidean inner product on the enveloping three-dimensional space. Further, semi-colons are used to denote surface covariant differentiation. Thus, for example,

$$\mathbf{a}_{\alpha;\beta} = \mathbf{a}_{\alpha,\beta} - \Gamma_{\alpha\beta}^\lambda \mathbf{a}_\lambda, \quad (5)$$

where $\Gamma_{\alpha\beta}^\lambda$ are the Christoffel symbols induced by the coordinates on ω . To simplify the notation we suppose that ω can be covered by a single coordinate patch. In the general case it may be covered by the union of a finite number of patches, this requiring minor adjustment of various formulae to be developed.

Equilibria are those configurations that render stationary the potential energy defined by

$$E = \int_\omega W(H, K; \theta^\alpha) da. \quad (6)$$

To accommodate the present constraint on area, we consider the augmented energy functional

$$E = \int_\Omega [JW(H, K; \theta^\alpha) + \lambda(\theta^\alpha)(J - 1)] dA, \quad (7)$$

where $\lambda(\theta^\alpha)$ is a Lagrange-multiplier field,

$$J = \sqrt{a/A} \quad (8)$$

is the local areal stretch induced by the map from a fixed reference surface Ω to the actual surface ω , and A is the value of a on Ω .

3 Stationarity, the shape equation and energy minimizers

To compute the variation of the energy it is necessary to have explicit formulas for the variational derivatives of J , H and K induced by the virtual displacement $\mathbf{u}(\theta^\alpha) = \dot{\mathbf{r}}$ of the equilibrium position field $\mathbf{r}(\theta^\alpha)$. We denote virtual displacements by a superposed dot. This is simply the derivative with respect to a parameter, ϵ say, that identifies configurations of the surface. The dot notation refers to the value of the derivative at a fixed value of the parameter, zero say, which we use to identify quantities associated with the particular equilibrium state considered. Thus, $\mathbf{u}(\theta^\alpha) = \frac{\partial}{\partial \epsilon} \mathbf{r}(\theta^\alpha; \epsilon)|_{\epsilon=0}$. Henceforth we intend that the same meaning should extend to any variable bearing a superposed dot.

Special roles are played by the tangential and normal variations, u^α and u respectively, in the general expression

$$\mathbf{u} = u^\alpha \mathbf{a}_\alpha + u \mathbf{n}. \quad (9)$$

We emphasize that this is the variation of the position of a fixed material point, identified by a fixed pair $\{\theta^\alpha\}$. In other words, we take the coordinates θ^α to be convected with the material.

The induced variation of the energy is

$$\dot{E} = \int_{\omega} [\dot{W} + (W + \lambda) \dot{J}/J] da, \quad (10)$$

where

$$\dot{W} = W_H \dot{H} + W_K \dot{K}. \quad (11)$$

Here and henceforth the subscripts H and K refer to partial derivatives. We note that, while the augmented functional may be considered to depend on both the position and Lagrange multiplier, regarded as independent fields, variation with respect to the latter merely returns the constraint and so need not be made explicit.

For example, under *tangential* variations we have [9]

$$\dot{J}/J = u^\alpha_{;\alpha}, \quad \dot{H} = u^\alpha H_{,\alpha} \quad \text{and} \quad \dot{K} = u^\alpha K_{,\alpha}, \quad (12)$$

wherein J , H and K are equilibrium fields. These furnish

$$\dot{W} = u^\alpha (W_H H_{,\alpha} + W_K K_{,\alpha}) \quad \text{and} \quad (W + \lambda) \dot{J}/J = [(W + \lambda) u^\alpha]_{;\alpha} - u^\alpha (W + \lambda)_{,\alpha}, \quad (13)$$

which may be combined with (10), (12)_{2,3} and Stokes' theorem to obtain the associated variation

$$\dot{E} = \int_{\omega} u^\alpha (W_H H_{,\alpha} + W_K K_{,\alpha} - W_{,\alpha} - \lambda_{,\alpha}) da + \int_{\partial\omega} (W + \lambda) u^\alpha \nu_\alpha ds, \quad (14)$$

where ν_α are the covariant components of the exterior unit normal to the edge $\partial\omega$, lying in the tangent plane of ω , as it is traversed in the direction of increasing arclength s . The associated Euler equation is equivalent to the vanishing of the parenthetical term in the first integral. To reduce this, we compute

$$W_{,\alpha} = W_H H_{,\alpha} + W_K K_{,\alpha} + \partial W / \partial \theta^\alpha, \quad (15)$$

where the partial derivative on the right is due to the explicit coordinate dependence in the function W . This arises from the possible non-uniformity of the film properties in the present context. Accordingly, the relevant Euler equation is expressible in the form

$$\lambda_{,\alpha} = -\partial W / \partial \theta^\alpha. \quad (16)$$

This yields $\lambda = \text{const.}$ in the special case of a film with properties that are uniform in the sense that W does not depend explicitly on the coordinates θ^α . A class of problems pertaining to non-uniform films is discussed in [6].

We note in passing that (infinitesimal) surface reparametrizations $\theta^\alpha \rightarrow \vartheta^\alpha(\epsilon)$ are formally subsumed under tangential variations. To see this we use the chain rule to compute the variation of $\mathbf{r}(\vartheta^\alpha(\epsilon))$ at $\epsilon = 0$, obtaining $\dot{\mathbf{r}} = \dot{\vartheta}^\alpha \mathbf{a}_\alpha$. This is of the form (9), with $u^\alpha = \dot{\vartheta}^\alpha$ and $u = 0$. However, the meaning intended in (9) is different. There we use the coordinates as labels for material points, and compute variations while holding

these fixed. The vanishing of the induced variation of the energy is simply the principle of virtual work in the present context. In the literature one sometimes finds statements to the effect that tangential variations are equivalent to reparametrizations of the surface and so may be suppressed on the basis of the belief that they are vacuous in the case of fluids. On the contrary, while it is appropriate to *impose* the invariance of the energy under arbitrary, hence infinitesimal, reparametrizations of the surface, in general this is not equivalent to rendering it stationary under tangential displacements u^α of material points. The issue is moot in the case of uniform films ($\partial W/\partial \theta^\alpha = 0$), for which the area constraint is typically expressed in global form in terms of a Lagrange multiplier that is uniform on ω . In this case tangential variations yield no new information. We refer to [9] for further discussion of this issue. In this work bona fide tangential variations (i.e., tangential virtual displacements of material points) play an essential role in the derivation of boundary conditions (Sect. 4).

For *normal* variations we have [9]

$$\dot{J}/J = -2Hu, \quad 2\dot{H} = \Delta u + u(4H^2 - 2K) \quad \text{and} \quad \dot{K} = 2KHu + (\tilde{b}^{\alpha\beta} u_{,\alpha})_{;\beta}, \quad (17)$$

where $\Delta(\cdot) = a^{\alpha\beta}(\cdot)_{;\alpha\beta}$ is the surface Laplacian, also known as the Beltrami operator. These lead to

$$(W + \lambda)\dot{J}/J = -2Hu(W + \lambda) \quad (18)$$

and, with some effort [9], to

$$\begin{aligned} \dot{W} = & u[\Delta(\tfrac{1}{2}W_H) + (W_K)_{;\beta\alpha}\tilde{b}^{\beta\alpha} + W_H(2H^2 - K) + 2KH W_K] \\ & + \tfrac{1}{2}(W_H a^{\alpha\beta} u_{,\alpha})_{;\beta} - \tfrac{1}{2}[(W_H)_{;\beta\alpha} a^{\alpha\beta} u]_{;\alpha} + (W_K \tilde{b}^{\alpha\beta} u_{,\alpha})_{;\beta} - [(W_K)_{;\beta\alpha} \tilde{b}^{\alpha\beta} u]_{;\alpha}. \end{aligned} \quad (19)$$

Thus, normal variations induce the energy variation

$$\begin{aligned} \dot{E} = & \int_{\omega} u[\Delta(\tfrac{1}{2}W_H) + (W_K)_{;\beta\alpha}\tilde{b}^{\beta\alpha} + W_H(2H^2 - K) + 2KH W_K - 2H(W + \lambda)]da \\ & + \int_{\partial\omega} [\tfrac{1}{2}W_H v^\alpha u_{,\alpha} - \tfrac{1}{2}(W_H)_{;\alpha} v^\alpha u + W_K \tilde{b}^{\alpha\beta} v_\beta u_{,\alpha} - (W_K)_{;\alpha} \tilde{b}^{\alpha\beta} v_\beta u]ds. \end{aligned} \quad (20)$$

Suppose the membrane, together with a rigid container, bounds a volume of incompressible liquid. We assume the membrane to be impermeable and regard the membrane and liquid as a closed system. The bulk incompressibility of the liquid is taken into account through the replacement

$$E \rightarrow E - \int_B P(\mathbf{X})[\det(\text{Grad } \chi) - 1]dV, \quad (21)$$

where $\chi(\mathbf{X})$ is a one-to-one deformation that maps a fixed configuration B of the bulk fluid to its current configuration, Grad is the gradient with respect to position $\mathbf{X} \in B$, $\mathbf{x} = \chi(\mathbf{X}; \epsilon)$ is the position of a material point in the current configuration, and $P(\mathbf{X})$ is a Lagrange multiplier field. Incompressibility is associated with the constraint $\det(\text{Grad } \chi) = 1$. This leads to the substitution

$$\dot{E} \rightarrow \dot{E} + \int_R \dot{\chi} \cdot \text{grad } P dv - \int_{\omega} u P da, \quad (22)$$

where R is the volume occupied by the liquid in its equilibrium configuration ($\omega \subset \partial R$) and grad is the gradient with respect to $\mathbf{x} \in R$. Accordingly, the Euler equations are $\text{grad } P = \mathbf{0}$, implying that P is uniform in R , and

$$\Delta(\tfrac{1}{2}W_H) + (W_K)_{;\beta\alpha}\tilde{b}^{\beta\alpha} + W_H(2H^2 - K) + 2KH W_K - 2H(W + \lambda) = P \quad \text{on } \omega. \quad (23)$$

It follows that P is mechanically equivalent to a net lateral pressure exerted on the membrane in the direction of its orientation $\mathbf{n}$.

It has been shown in [10] that a further necessary condition for an equilibrium state to be energy *minimizing*, in addition to (16) and (23), is

$$\tfrac{1}{4}W_{HH} + \varsigma W_{HK} + \varsigma^2 W_{KK} > 0 \quad (24)$$

at all points of the film, where

$$\varsigma = \tilde{b}^{\alpha\beta} b_\alpha b_\beta, \quad (25)$$

and the b_β are arbitrary subject to the normalization condition $a^{\alpha\beta} b_\alpha b_\beta = 1$.

For bilayers that have no natural orientation the energy function W satisfies the symmetry relation $W(H, K; \theta^\alpha) = W(-H, K; \theta^\alpha)$ [11]. A well-known example due to Helfrich [12] is

$$W = kH^2 + \bar{k}K, \quad (26)$$

wherein k and $\bar{k}$ are empirical constants, and pertains to films with uniform properties. This is compatible with (24) if and only if $k > 0$, while $\bar{k}$ is unrestricted, and the shape equation reduces to

$$k[\Delta H + 2H(H^2 - K)] - 2\lambda H = P. \quad (27)$$

The Helfrich function may be motivated by observing that the thickness t of the bilayer furnishes a local length scale. Then, because W is defined pointwise, it is expressible in the form $W = E\bar{W}(\bar{H}, \bar{K}; \theta^\alpha)$ [13], where E is a constant with the same physical dimensions as W , $\bar{W}$ is a dimensionless function, $\bar{H} = tH$ is the dimensionless mean curvature and $\bar{K} = t^2K$ is the dimensionless Gaussian curvature. We have in mind applications characterized by the feature that the thickness is everywhere much smaller than the smallest principal radius of curvature in any configuration of the membrane. Thus, $|\bar{H}| \ll 1$ and $|\bar{K}| \ll 1$. Developing the function $\bar{W}$ in a Taylor expansion in terms of the (small) dimensionless curvature $\bar{b}_{\alpha\beta} = tb_{\alpha\beta}$ about a state of zero curvature, and retaining terms up to quadratic order, we obtain the expression $\bar{W} = a\bar{H} + b\bar{H}^2 + c\bar{K}$, in which the coefficients may depend on the coordinates. These are constants if the film is uniform. Bilayer symmetry requires that $\bar{W}$ be an even function of $\bar{H}$; accordingly, $a = 0$ and (26) follows.

In general, bilayer symmetry implies that $P = 0$ if the membrane is flat anywhere. For, the odd-order derivatives of W with respect to H vanish at zero curvature and (23) reduces to $P = 0$. The uniformity of P then implies that it vanishes everywhere.

4 Edge conditions

With (16) and (23) satisfied the variation of the energy reduces to $\dot{E} = \dot{E}_B$, where

$$\dot{E}_B = B_t + B_n, \quad (28)$$

and

$$B_t = \int_{\partial\omega} (W + \lambda) u^\alpha v_\alpha ds, \quad (29)$$

$$B_n = \int_{\partial\omega} [\tfrac{1}{2} W_H v^\alpha u_{,\alpha} - \tfrac{1}{2} (W_H)_{,\alpha} v^\alpha u + W_K \tilde{b}^{\alpha\beta} v_\beta u_{,\alpha} - (W_K)_{,\alpha} \tilde{b}^{\alpha\beta} v_\beta u] ds, \quad (30)$$

respectively, are the contributions to the boundary working arising from tangential and normal variations. To reduce the latter to a usable form it is necessary to express the derivatives $u_{,\alpha}$ of a normal variation in terms of its independent arclength and normal derivatives $u'(s)$ and $u_{,v}$ on $\partial\omega$. These are the restrictions to $\partial\omega$ of $\tau^\alpha u_{,\alpha}$ and $v^\alpha u_{,\alpha}$, respectively, where τ is the unit tangent to $\partial\omega$, pointing in the direction of increasing arclength. Let $\theta^\alpha(s)$ be the parametrization of $\partial\omega$. Then,

$$\mathbf{v} = v_\alpha \mathbf{a}^\alpha = \tau \times \mathbf{n}, \quad (31)$$

where

$$\tau = \frac{d}{ds} \mathbf{r}(\theta^\alpha(s)) = \tau^\alpha \mathbf{a}_\alpha \quad \text{and} \quad \tau^\alpha = d\theta^\alpha/ds. \quad (32)$$

The required expression follows from the orthonormality of $\{\mathbf{v}, \tau\}$. Thus [14],

$$u_{,\alpha} = \tau_\alpha u' + v_\alpha u_{,v}. \quad (33)$$

Combining this with [5]

$$\tilde{b}^{\alpha\beta} = 2Ha^{\alpha\beta} - b^{\alpha\beta} \quad (34)$$

and

$$a^{\alpha\beta} = \tau^\alpha \tau^\beta + v^\alpha v^\beta \quad (35)$$

results in

$$a^{\alpha\beta} u_{,\alpha} = \tau^\beta u' + v^\beta u_{,v} \quad (36)$$

and

$$W_K \tilde{b}^{\alpha\beta} v_\beta u_{,\alpha} = u(\tau W_K)' - (\tau W_K u)' + (2H - \kappa_v) W_K u_{,v}. \quad (37)$$

Here,

$$\tau = b^{\alpha\beta} \tau_\alpha v_\beta \quad (38)$$

is the *twist* of the surface ω on the $\mathbf{v}$, $\boldsymbol{\tau}$ -axes, and

$$\kappa_v = b^{\alpha\beta} v_\alpha v_\beta \quad (39)$$

is its *normal* curvature in the direction of $\mathbf{v}$. Thus, for $\partial\omega$ piecewise smooth in the sense that $\mathbf{a}_\alpha$ is continuous there, while $\bar{\mathbf{r}}(s) = \mathbf{r}(\theta^\alpha(s))$ is piecewise differentiable (so that $\boldsymbol{\tau}$ can have a finite number of jumps), we obtain

$$B_n = \int_{\partial\omega} [(\tau W_K)' - \frac{1}{2} v^\beta (W_H)_{,\beta} - (W_K)_{,\beta} \tilde{b}^{\alpha\beta} v_\alpha] u ds + \int_{\partial\omega} (\frac{1}{2} W_H + \kappa_\tau W_K) u_{,v} ds + \sum u W_K[\tau], \quad (40)$$

where the square bracket in the summand identifies the forward jump of the enclosed quantity at a corner of $\partial\omega$ (a point where $\boldsymbol{\tau}$ is discontinuous), and

$$\kappa_\tau = b_{\alpha\beta} \tau^\alpha \tau^\beta = 2H - \kappa_v \quad (41)$$

is the normal curvature of ω in the direction of $\boldsymbol{\tau}$. The twist and normal curvatures are simply the components of the curvature tensor $\mathbf{b} = b_{\alpha\beta} \mathbf{a}^\alpha \otimes \mathbf{a}^\beta$ on the $\mathbf{v}$, $\boldsymbol{\tau}$ -axes; i.e.,

$$\mathbf{b} = \kappa_v \mathbf{v} \otimes \mathbf{v} + \kappa_\tau \boldsymbol{\tau} \otimes \boldsymbol{\tau} + \tau(\mathbf{v} \otimes \boldsymbol{\tau} + \boldsymbol{\tau} \otimes \mathbf{v}). \quad (42)$$

Some conceptual clarity is gained by expressing u and $u_{,v}$ in terms of the virtual displacement $\mathbf{u}$ and its normal derivative $\mathbf{u}_{,v} = v^\alpha \mathbf{u}_{,\alpha}$. To this end we use $u = \mathbf{u} \cdot \mathbf{n}$ to obtain

$$u_{,v} = v^\alpha (\mathbf{u} \cdot \mathbf{n})_{,\alpha} = \mathbf{n} \cdot \mathbf{u}_{,v} + \mathbf{u} \cdot \mathbf{n}_{,v}, \quad (43)$$

where

$$\mathbf{n}_{,v} = v^\alpha \mathbf{n}_{,\alpha} = -v^\alpha b_\alpha^\beta \mathbf{a}_\beta. \quad (44)$$

The latter may be simplified by substituting

$$\mathbf{a}_\beta = \tau_\beta \boldsymbol{\tau} + v_\beta \mathbf{v}, \quad (45)$$

yielding

$$\mathbf{n}_{,v} = -\tau \boldsymbol{\tau} - \kappa_v \mathbf{v}. \quad (46)$$

Further, it is possible to show that [15]

$$\dot{\mathbf{n}} = -(\mathbf{n} \cdot \mathbf{u}_{,v}) \mathbf{v} - (\mathbf{n} \cdot \mathbf{u}') \boldsymbol{\tau}, \quad (47)$$

where $\dot{\mathbf{n}}$ is the variation of $\mathbf{n}$. Because the latter is a unit vector in all configurations of the surface, it follows that $\dot{\mathbf{n}} = \boldsymbol{\omega} \times \mathbf{n}$ for some vector $\boldsymbol{\omega}$. Thus,

$$-\mathbf{n} \cdot \mathbf{u}_{,v} = \boldsymbol{\tau} \cdot \boldsymbol{\omega} \quad (48)$$

and hence

$$u_{,v} = -\boldsymbol{\tau} \cdot \boldsymbol{\omega} - \mathbf{b}\mathbf{v} \cdot \mathbf{u}. \quad (49)$$

We also note the relations

$$\mathbf{n} \cdot \mathbf{u}' = \mathbf{v} \cdot \boldsymbol{\omega} \quad \text{and} \quad u' = \mathbf{v} \cdot \boldsymbol{\omega} - \mathbf{b}\boldsymbol{\tau} \cdot \mathbf{u}, \quad (50)$$

which are derived similarly.

The foregoing may be used to reduce (28) to the compact form

$$\dot{E}_B = \int_{\partial\omega} (F_v \mathbf{v} + F_\tau \boldsymbol{\tau} + F_n \mathbf{n}) \cdot \mathbf{u} ds - \int_{\partial\omega} M \boldsymbol{\tau} \cdot \boldsymbol{\omega} ds + \sum \mathbf{f}_i \cdot \mathbf{u}_i, \quad (51)$$

where

$$M = \frac{1}{2} W_H + \kappa_\tau W_K \quad (52)$$

is the bending couple applied to ω per unit length of $\partial\omega$,

$$F_v = W + \lambda - \kappa_v M, \quad F_\tau = -\tau M \quad \text{and} \quad F_n = (\tau W_K)' - (\frac{1}{2} W_H)_{,v} - (W_K)_{,\beta} \tilde{b}^{\alpha\beta} v_\alpha, \quad (53)$$

respectively, are the $\mathbf{v}$ -, $\boldsymbol{\tau}$ - and $\mathbf{n}$ -components of the force per unit length applied to $\partial\omega$, and

$$\mathbf{f}_i = W_K[\tau]_i \mathbf{n} \quad (54)$$

is the force applied to the film at the i th corner of $\partial\omega$.

4.1 Wetting and the adhesion energy

We consider the problem of a volume of liquid with uniform properties bounded by the film ω and a rigid wall Γ . The boundary $\partial\omega$ is a simple closed curve on Γ . Conventionally, wetting of the wall is accommodated by appending the phenomenological adhesion energy

$$E_{\Gamma^*} = -\sigma A_{\Gamma^*} \quad (55)$$

to the total energy E , where A_{Γ^*} is the surface area of the portion $\Gamma^* \subset \Gamma$ of the wall wetted by the volume of liquid and σ is an empirical constant. Positive values of σ promote wetting; i.e., an increase of A_{Γ^*} , while negative values penalize it. For $\sigma > 0$, the energy is bounded below provided that A_{Γ^*} is finite.

Here we allow the film/substrate interaction to be non-uniform. To accommodate this we assume σ —the adhesion energy per unit area—to be an assigned function of position $\mathbf{x} \in \Gamma$. The net adhesion energy is thus given by

$$E_{\Gamma^*} = - \int_{\Gamma^*} \sigma d\mathbf{a}. \quad (56)$$

The variation of this energy induced by the movement of $\partial\omega$ on Γ is

$$\dot{E}_{\Gamma^*} = - \lim_{\epsilon \rightarrow 0} \frac{1}{\epsilon} \left[\int_{\Gamma_\epsilon^*} \sigma(\mathbf{x}) d\mathbf{a} - \int_{\Gamma^*} \sigma(\mathbf{x}) d\mathbf{a} \right], \quad (57)$$

where Γ_ϵ^* is the wetted surface associated with the configuration $\mathbf{r}(\theta^\alpha; \epsilon)$ of the membrane and $\Gamma^* = \Gamma_0^*$ is that of the equilibrium configuration, corresponding to $\epsilon = 0$. The variation $\dot{E}_{\Gamma^*}$ is generated by a virtual

Fig. 1 Wetting and de-wetting of a rigid wall by the movement of $\partial\omega$

displacement $\mathbf{u} \in T_\Gamma$, where T_Γ is the tangent plane to Γ at a point of $\partial\omega$. We take $\epsilon > 0$ without loss of generality. Now, observing that

$$\Gamma_\epsilon^* = \{\Gamma_\epsilon^* \cap \Gamma^*\} \cup \{\Gamma_\epsilon^* \cap \bar{\Gamma}^*\} \quad \text{and} \quad \Gamma^* = \{\Gamma^* \cap \Gamma_\epsilon^*\} \cup \{\Gamma^* \cap \bar{\Gamma}_\epsilon^*\}, \quad (58)$$

where $\bar{\Gamma}^*$ and $\bar{\Gamma}_\epsilon^*$ respectively are the complements of Γ^* and Γ_ϵ^* with respect to Γ , we obtain

$$\int_{\Gamma_\epsilon^*} \sigma(\mathbf{x}) da - \int_{\Gamma^*} \sigma(\mathbf{x}) da = \int_{\Gamma_\epsilon^* \cap \bar{\Gamma}^*} \sigma(\mathbf{x}) da - \int_{\Gamma^* \cap \bar{\Gamma}_\epsilon^*} \sigma(\mathbf{x}) da, \quad (59)$$

where $\Gamma_\epsilon^* \cap \bar{\Gamma}^*$ is the additional portion of Γ that is wetted due to the advancement of $\partial\omega$. Accordingly, in the associated integral we have $da = \epsilon \mathbf{t} \cdot \mathbf{u} ds$ to leading order, where $\mathbf{t} \cdot \mathbf{u} \geq 0$,

$$\mathbf{t} \in \text{Span}\{\mathbf{v}, \mathbf{n}\} \quad (60)$$

is the exterior unit normal to Γ^* lying in T_Γ , and s measures arclength on $\partial\omega$ (Fig. 1). The part $\Gamma^* \cap \bar{\Gamma}_\epsilon^*$ is de-wetted in this process, so that $\mathbf{t} \cdot \mathbf{u} \leq 0$ and $da = -\epsilon \mathbf{t} \cdot \mathbf{u} ds$ to leading order. Hence the estimate

$$\int_{\Gamma_\epsilon^*} \sigma(\mathbf{x}) da - \int_{\Gamma^*} \sigma(\mathbf{x}) da = \epsilon \int_{\partial\omega} \sigma(\mathbf{x}(s)) \mathbf{t} \cdot \mathbf{u} ds + o(\epsilon), \quad (61)$$

where $\mathbf{x}(s)$ is the arclength parametrization of $\partial\omega \cap \Gamma$, and (57) furnishes

$$\dot{E}_{\Gamma^*} = - \int_{\partial\omega} \sigma \mathbf{t} \cdot \mathbf{u} ds. \quad (62)$$

This result covers the cases $\Gamma^* \subset \Gamma_\epsilon^*$ and $\Gamma_\epsilon^* \subset \Gamma^*$ corresponding to $\Gamma^* \cap \bar{\Gamma}_\epsilon^* = \emptyset$ and $\Gamma_\epsilon^* \cap \bar{\Gamma}^* = \emptyset$, respectively.

Because $\partial\omega \subset \Gamma$ we have $T_\Gamma = \text{Span}\{\mathbf{t}, \boldsymbol{\tau}\}$, and any variation $\mathbf{u} \in T_\Gamma$ is expressible in the form

$$\mathbf{u} = u_t \mathbf{t} + u_\tau \boldsymbol{\tau}. \quad (63)$$

For these the boundary working, including the effects of wetting, reduces to

$$\dot{E}_B = \int_{\partial\omega} [(F_v \cos \gamma + F_n \sin \gamma - \sigma) u_t + F_\tau u_\tau] ds - \int_{\partial\omega} M \boldsymbol{\tau} \cdot \boldsymbol{\omega} ds + \sum \mathbf{f}_i \cdot \mathbf{u}_i, \quad (64)$$

where γ is the contact angle ($\cos \gamma = \mathbf{v} \cdot \mathbf{t}$ and $\sin \gamma = \mathbf{n} \cdot \mathbf{t}$).

4.2 Hard anchoring

The anchoring of the lipids is said to be *hard* if $\mathbf{n}$ is assigned on $\partial\omega$. This models situations in which deviations from the assigned values are energetically disfavored. This is expected to be the case when the wall Γ has a natural structural symmetry or one that is induced by polishing. For example, an isotropic wall may acquire a preferred orientation through abrasion. The lipids may then become aligned with the resulting microscopic grooves, whose trajectories confer an orientation to the wall. If the lipids become embedded in the grooves, then it is to be expected that displacements transverse to the grooves would also be disfavored.

The example described, to which attention is here restricted, is idealized by the constraints (Fig. 2)

$$\mathbf{n} = \mathbf{t}, \mathbf{t} \text{ assigned on } \partial\omega; \quad u_\tau = 0, \quad (65)$$

while u_t is arbitrary. We note that in this case $u_t = u$, the restriction of the *normal* variation to $\partial\omega$.

We illustrate this class of problems for grooves that coincide with a family of congruent helices on a right circular cylinder Γ of radius a . Thus, let $\{r, \theta, z\}$ be the usual cylindrical polar coordinates and $\{\mathbf{e}_r, \mathbf{e}_\theta, \mathbf{k}\}$ the associated orthonormal basis; i.e., $\mathbf{e}_r(\theta)$ is the exterior unit normal to the cylindrical surface at azimuth θ , $\mathbf{k}$ is aligned with the axis of the cylinder, and $\mathbf{e}_\theta(\theta) = \mathbf{k} \times \mathbf{e}_r = \mathbf{e}'_r(\theta)$ is a unit tangent to a circle of latitude. A typical helix is described in parametric form by

$$\mathbf{x}(\xi) = a\mathbf{e}_r(\theta(\xi)) + z(\xi)\mathbf{k}; \quad \theta(\xi) = \xi/c, \quad z(\xi) = b\theta(\xi), \quad (66)$$

where ξ measures arclength on the helix, $b(>0)$ is the (constant) pitch, and $c = \sqrt{a^2 + b^2}$. The unit tangent to the helix is

$$\mathbf{t} = \mathbf{x}'(\xi) = (a/c)\mathbf{e}_\theta + (b/c)\mathbf{k}. \quad (67)$$

Because $\boldsymbol{\tau} \in T_\Gamma$, (65)₁ implies that $\mathbf{v}$ is normal to T_Γ and hence parallel to $\mathbf{e}_r$. Further, $\mathbf{v}$ is directed away from the film, and thus into the cylinder. Accordingly,

$$\mathbf{v} = -\mathbf{e}_r, \quad \boldsymbol{\tau} = \mathbf{n} \times \mathbf{v} = (a/c)\mathbf{k} - (b/c)\mathbf{e}_\theta. \quad (68)$$

The variation of $\mathbf{n}$ is given by (65)₁ and (67). This yields $\dot{\mathbf{n}} = -(a/c)\mathbf{e}_r\dot{\theta}$, where $\dot{\theta}$ is the variation of the azimuth of a material point on $\partial\omega$ induced by a variation $\mathbf{u} \in T_\Gamma$ of its position. We have $\dot{\mathbf{n}} = \boldsymbol{\omega} \times \mathbf{n}$, where $\boldsymbol{\omega} = (a/c)\dot{\theta}\boldsymbol{\tau}$. Further, $\mathbf{u} = \dot{\mathbf{r}} = \dot{\mathbf{x}}$, where $\dot{\mathbf{x}} = \dot{\xi}\mathbf{t}$. This follows from the fact that points of the membrane belonging to $\partial\omega$ are constrained to follow the trajectories of the helices (cf. (65)₃). Thus, $\mathbf{u} = u\mathbf{n}$, where $u = \dot{\xi} = c\dot{\theta}$, yielding $\boldsymbol{\omega} \cdot \boldsymbol{\tau} = (a/c^2)u$. Next, we observe that (50)₂ yields $u'(s) = 0$, and thus $u = \text{const.}$ on $\partial\omega$. Using these results with (64), we find that the energy is stationary only if the overall force balance

$$\int_{\partial\omega} [F_n - (a/c^2)M]ds = 0 \quad (69)$$

is satisfied. Here we assume that no bulk fluid is present ($\sigma = 0$, $P = 0$). The non-standard global nature of this condition is due to the fact that only constant normal variations on $\partial\omega$ are admitted by the constraints. This effectively means that $\partial\omega$ undergoes a uniform parallel motion on Γ in the course of a virtual displacement.

Fig. 2 Interaction of membrane, substrate and bulk liquid

The right circular helicoid [16] furnishes a solution to the problem of a uniform bilayer adjoining the cylinder. To establish this we show that membrane configurations of the form

$$\mathbf{r}(\theta^\alpha) = r\mathbf{e}_r(\theta) + z(\theta)\mathbf{k}; \quad z(\theta) = p\theta, \quad \theta^1 = r, \quad \theta^2 = \theta, \quad (70)$$

with p a suitable constant, satisfy the equilibrium and boundary conditions. Direct computation yields the orientation and curvature-tensor fields

$$\mathbf{n} = (r\mathbf{k} - p\mathbf{e}_\theta)/\sqrt{r^2 + p^2} \quad \text{and} \quad \mathbf{b} = \frac{-p}{r^2 + p^2}(\mathbf{e}_r \otimes \mathbf{i} + \mathbf{i} \otimes \mathbf{e}_r), \quad \text{where} \quad \mathbf{i} = (r\mathbf{e}_\theta + p\mathbf{k})/\sqrt{r^2 + p^2}. \quad (71)$$

Therefore,

$$H = 0, \quad K = -p^2/(r^2 + p^2)^2, \quad (72)$$

and, for bilayers, the shape equation (23) (with $P = 0$) reduces to

$$v_{;\beta}^\beta = 0, \quad \text{where} \quad v^\beta = (W_K)_{,\alpha} \tilde{b}^{\beta\alpha}. \quad (73)$$

Here we have used bilayer symmetry with (72)₁ to conclude that odd-order derivatives of W with respect to H vanish and hence that W_H vanishes identically. We have also used the Mainardi–Codazzi equations of surface theory in the form $\tilde{b}^{\beta\alpha}_{;\beta} = 0$ [5]. For uniform bilayers it follows from (72)₁ that $(W_K)_{,\alpha} = W_{KK} K_{,\alpha}$. Thus, (73)₂ yields

$$v^\beta = -W_{KK} \mathbf{a}^\beta \cdot \mathbf{b}(\nabla K), \quad (74)$$

where $\mathbf{a}^\beta = a^{\beta\alpha} \mathbf{a}_\alpha$ are the dual basis vectors on the tangent plane to ω and $\nabla(\cdot) = (\cdot)_{,\alpha} \mathbf{a}^\alpha$ is the (tangential) surface gradient on ω . Straightforward calculations lead to $v^1 = 0$ and to the conclusion that v^2 is a function of θ^1 alone. Then, $v_{;\beta}^\beta = a^{-1/2}(a^{1/2}v^\beta)_{,\beta}$, where $a = \det(a_{\alpha\beta}) = r^2 + p^2$, vanishes and (73)₁ is identically satisfied.

Turning now to the boundary conditions we note that, according to (65)₁, the curve $\partial\omega \subset \Gamma$ is the orthogonal trajectory of the helix described by (66). This too is a helix, on which arclength is given by $s = q\theta$ for some constant q (cf. (66)). We impose $q < 0$ to ensure that an increment in s corresponds to a decrement in θ . Putting $r = a$ in (70), we obtain the parametrization

$$\mathbf{r}(s) = a\mathbf{e}_r(s/q) + s(p/q)\mathbf{k} \quad (75)$$

of $\partial\omega$. The unit tangent is

$$\boldsymbol{\tau} = \mathbf{r}'(s) = (a/q)\mathbf{e}_\theta + (p/q)\mathbf{k}; \quad \text{hence,} \quad q = -\sqrt{a^2 + p^2}. \quad (76)$$

This is orthogonal to $\mathbf{t}$, as required by (65)₁, if and only if

$$pb = -a^2, \quad (77)$$

and thus $p < 0$. These results yield $\mathbf{v} = \boldsymbol{\tau} \times \mathbf{n} = -\mathbf{e}_r$, while (68) and (76) furnish

$$p/q = a/c \quad \text{and} \quad a/q = -b/c. \quad (78)$$

From (68)₁ and (71)₂, the restriction to $\partial\omega$ of the normal curvature $\kappa_v (= \mathbf{v} \cdot \mathbf{b}\mathbf{v})$ vanishes. Accordingly, Eqs. (41) and (52) imply that M vanishes on $\partial\omega$. Further, (53)₃ and (68)₁ imply that the normal force density reduces to

$$F_n = (\tau W_K)' + \frac{1}{2}\mathbf{e}_r \cdot \nabla(W_H) + (W_K)_{,\beta} b^{\beta\alpha} v_\alpha, \quad (79)$$

where $\tau (= \boldsymbol{\tau} \cdot \mathbf{b}\mathbf{v}) = -p/q^2$ is the restriction to $\partial\omega$ of the membrane twist. From (72)₁ we have $\nabla(W_H) = W_{HK} \nabla K$ in which W_{HK} vanishes identically by virtue of bilayer symmetry. In the same way, $(\tau W_K)'$ reduces to $\tau W_{KK} K'$. This vanishes identically because K is constant on $\partial\omega \subset \Gamma$ (cf. (72)₂ with $r = a$). Finally, the third term in (79) is $-\nabla(W_K) \cdot \mathbf{b}\mathbf{e}_r$, which is proportional to $W_{KK} \mathbf{i} \cdot \nabla K$. This vanishes because ∇K is parallel to $\mathbf{e}_r$ and thus orthogonal to $\mathbf{i}$ (cf. (71)₃). Accordingly, F_n also vanishes and the force balance (69) is identically satisfied.

4.3 Conical anchoring

Conical anchoring models the interaction of the lipid molecules with a wall Γ having isotropic properties [7, 8]. Let $\mathbf{N}$ be the unit normal to the wall at a point of $\partial\omega$. Typically [8] this interaction is such that it is energetically costly for configurations of $\mathbf{n}$ to deviate from a cone with axis $\mathbf{N}$. Conical anchoring idealizes this situation by the constraint (see Fig. 2)

$$\mathbf{n} \cdot \mathbf{N} = \cos \gamma \quad (80)$$

in which γ is assigned.

If Γ is a plane, then $\dot{\mathbf{N}}$ vanishes at a material point of $\partial\omega$ for all variations $\mathbf{u} \in T_\Gamma$ of its position. If the membrane/wall interaction is uniform in the sense that γ is constant on Γ , then $\dot{\mathbf{n}} \cdot \mathbf{N} = 0$. In particular, $\dot{\mathbf{n}} = \boldsymbol{\omega} \times \mathbf{n}$ with $\boldsymbol{\omega} = \phi \mathbf{N}$, corresponding to an infinitesimal rotation of $\mathbf{n}$ by amount ϕ around the axis $\mathbf{N}$. It follows that $\boldsymbol{\tau} \cdot \boldsymbol{\omega}$ vanishes identically and the stationarity condition $\dot{E} = 0$ for equilibria yields the natural boundary conditions

$$F_v \cos \gamma + F_n \sin \gamma = \sigma \quad \text{and} \quad F_\tau = 0 \quad \text{on} \quad \partial\omega, \quad (81)$$

the first of which generalizes the classical Young equation $\lambda \cos \gamma = \sigma$ of classical capillarity theory [17], to which it reduces if the bending energy vanishes; the second equation reduces to an identity.

If Γ is curved, then $\dot{\mathbf{N}}$ does not vanish for general $\mathbf{u} \in T_\Gamma$. Instead, we have $\dot{\mathbf{N}} = \boldsymbol{\Omega} \times \mathbf{N}$ for some vector $\boldsymbol{\Omega}$ and the variation of (80) yields $\boldsymbol{\omega} \times \mathbf{n} \cdot \mathbf{N} + \mathbf{n} \cdot \boldsymbol{\Omega} \times \mathbf{N} = -(\sin \gamma) \dot{\gamma}$, where we now admit the possibility of a non-uniform film/wall interaction; i.e., γ is an assigned function of $\mathbf{x} \in \Gamma$. In this case a non-trivial variation of γ on $\partial\omega$ is induced by the movement of $\partial\omega$ relative to points of Γ in accordance with $\dot{\gamma} = \nabla_\Gamma \gamma \cdot \mathbf{u}$, where ∇_Γ is the tangential surface gradient on Γ . Using $\mathbf{N} \times \mathbf{n} = \sin \gamma \boldsymbol{\tau}$ (Fig. 2) and assuming $\sin \gamma \neq 0$, we derive

$$\boldsymbol{\tau} \cdot (\boldsymbol{\omega} - \boldsymbol{\Omega}) = \nabla_\Gamma \gamma \cdot \mathbf{u} \quad \text{on} \quad \partial\omega. \quad (82)$$

To interpret this condition in terms of the geometry of Γ we use $d\mathbf{N} = -\mathbf{B}d\mathbf{x}$ for $d\mathbf{x} \in T_\Gamma$, where $\mathbf{B}$ is the (symmetric) curvature tensor of Γ . This maps T_Γ to itself. Then,

$$\dot{\mathbf{N}} = -\mathbf{B}\mathbf{u} \quad (83)$$

is the variation of $\mathbf{N}$ induced by the virtual displacement $\mathbf{u} \in T_\Gamma$ of $\partial\omega$ on Γ . Comparing this to $\dot{\mathbf{N}} = \boldsymbol{\Omega} \times \mathbf{N}$ yields

$$\Omega_t = \mathbf{B}\boldsymbol{\tau} \cdot \mathbf{u} \quad \text{and} \quad \Omega_\tau = -\mathbf{B}\mathbf{t} \cdot \mathbf{u}, \quad (84)$$

where $\boldsymbol{\tau} = \mathbf{N} \times \mathbf{t}$, $\Omega_t = \mathbf{t} \cdot \boldsymbol{\Omega}$ and $\Omega_\tau = \boldsymbol{\tau} \cdot \boldsymbol{\Omega}$; Eq. (82) becomes

$$\boldsymbol{\tau} \cdot \boldsymbol{\omega} = (\nabla_\Gamma \gamma - \mathbf{B}\mathbf{t}) \cdot \mathbf{u}. \quad (85)$$

Combining this with (63) and (64) furnishes the natural boundary conditions

$$F_v \cos \gamma + F_n \sin \gamma - M\mathbf{t} \cdot (\nabla_\Gamma \gamma - \mathbf{B}\mathbf{t}) = \sigma, \quad F_\tau - M\boldsymbol{\tau} \cdot (\nabla_\Gamma \gamma - \mathbf{B}\mathbf{t}) = 0, \quad (86)$$

the first of these again reducing to the classical Young equation in the absence of bending energy; the second to an identity.

4.4 Example

These conditions are illustrated by solving the Helfrich shape equation (27) with $P = 0$ on the unbounded domain $r \geq a (> 0)$, where r is the radius in a system of cylindrical polar coordinates (see Sect. 4.2). We take Γ to be a hydrophobic right circular cylinder ($\mathbf{N} = \mathbf{e}_r$) of radius a on which σ is a negative constant, so that wetting by the bulk liquid is energetically disfavored. Consistent with this we assign $\gamma = \pi/2$ in (86)_{1,2}. This yields $\mathbf{n} = \mathbf{k}$ at the wall, implying that the hydrophobic tail groups of the bilayer are in contact with the cylinder and thus shielded from the surrounding aqueous phase. Further, the curvature of the cylinder is easily found to be

$$\mathbf{B} = -a^{-1} \mathbf{e}_\theta \otimes \mathbf{e}_\theta. \quad (87)$$

Fig. 3 Meridian of a surface of revolution

We seek an axisymmetric solution in the class of surfaces of revolution parametrized by meridional arclength s and azimuthal angle θ . Thus,

$$\mathbf{r}(s, \theta) = r(s)\mathbf{e}_r(\theta) + z(s)\mathbf{k}, \quad (88)$$

where $r(s)$ is the radius from the axis of symmetry and $z(s)$ is the elevation above a base plane. Meridians and parallels of latitude are the curves on which θ and s , respectively, are constant. Because s measures arclength along meridians, we have

$$(r')^2 + (z')^2 = 1. \quad (89)$$

The surface coordinates are taken to be $\theta^1 = s$ and $\theta^2 = \theta$. The induced tangent vectors are

$$\mathbf{a}_1 = r'\mathbf{e}_r + z'\mathbf{k} \quad \text{and} \quad \mathbf{a}_2 = r\mathbf{e}_\theta, \quad (90)$$

and it follows from (89) that there is $\psi(s)$ such that

$$r'(s) = \cos \psi \quad \text{and} \quad z'(s) = \sin \psi. \quad (91)$$

Because $\mathbf{a}_1$ is orthogonal to a parallel of latitude, we identify it with $-\mathbf{v}$ (Fig. 3). Accordingly,

$$\mathbf{v} = -\cos \psi \mathbf{e}_r - \sin \psi \mathbf{k}, \quad \boldsymbol{\tau} = -\mathbf{e}_\theta \quad \text{and} \quad \mathbf{n} = \cos \psi \mathbf{k} - \sin \psi \mathbf{e}_r. \quad (92)$$

The metric and dual metric are $(a_{\alpha\beta}) = \text{diag}(1, r^2)$ and $(a^{\alpha\beta}) = \text{diag}(1, r^{-2})$, respectively, and the latter may be used to compute

$$\mathbf{a}^1 = -\mathbf{v} \quad \text{and} \quad \mathbf{a}^2 = r^{-1}\mathbf{e}_\theta. \quad (93)$$

To obtain the components of curvature we use (4)₁ and (5) with

$$\mathbf{a}_{1,1} = \psi' \mathbf{n}, \quad \mathbf{a}_{1,2} = \mathbf{a}_{2,1} = \cos \psi \mathbf{e}_\theta \quad \text{and} \quad \mathbf{a}_{2,2} = -r\mathbf{e}_r, \quad (94)$$

obtaining $(b_{\alpha\beta}) = \text{diag}(\psi', r \sin \psi)$. Combining this with (42) and (92) leads to

$$\kappa_v = \psi', \quad \kappa_\tau = r^{-1} \sin \psi \quad \text{and} \quad \tau = 0. \quad (95)$$

The sum of the normal curvatures is twice the mean curvature $H(s)$. This furnishes the differential equation

$$r\psi' = 2rH - \sin \psi. \quad (96)$$

Their product yields the Gaussian curvature $K(s)$, which is thus given by

$$K = H^2 - (H - r^{-1} \sin \psi)^2. \quad (97)$$

The shape equation (27), with $P = 0$, simplifies to [10]

$$L' = r[(2\lambda/k)H - 2H(H - r^{-1} \sin \psi)^2], \quad (98)$$

with

$$H' = r^{-1}L. \quad (99)$$

The system to be solved thus consists of (91)_{1,2}, (96), (98) and (99), for the unknowns r , z , ψ , H and L .

For the conditions discussed in the text preceding (87), the boundary condition (86)₂ is identically satisfied while (86)₁ reduces to $F_n = \sigma$, where $F_n = -kH_{,v}$. Further, the condition $\gamma = \pi/2$ requires that ψ vanish at the boundary, defined here by $s = 0$. Thus,

$$r(0) = a, \quad H'(0) = \sigma/k, \quad \psi(0) = 0 \quad \text{and} \quad z(0) = 0. \quad (100)$$

The last of these resolves the trivial non-uniqueness associated with a rigid translation of the film along the axis of the cylinder. We observe that, for $\sigma = 0$, a surface with vanishing H and ψ ; i.e., a horizontal plane, furnishes a solution to the problem. Thus, if the surface tends asymptotically to a plane in the far-field, then for non-zero σ any significant deviation from planarity can be expected to be localized near the boundary ($s = 0$). Accordingly, for purposes of numerical analysis we also assign $H(S) = 0$ for some $S > 0$ and solve the boundary-value problem on a succession of domains corresponding to a sequence of increasing values of S . This sequence is terminated when the solution converges on the domain of the last-solved boundary-value problem. This ensures that $H(s)$ tends to zero in the far field. From (96) this condition is seen to ensure that ψ tends to a constant value for large r , and hence, by virtue of (91)₁, for large s . The curvatures κ_v and κ_τ , and hence the Gaussian curvature K , also vanish in this limit. In this way we model a film that is asymptotically flat at large distances from the cylinder. This in turn is consistent with the assumption of vanishing lateral pressure. Further, (53) implies that the traction on a circle of latitude tends asymptotically to λ in the far field. Assuming this to be tensile, we consider λ to be an assigned positive constant.

Equation (98) contains the natural length scale μ^{-1} , where

$$\mu = \sqrt{2\lambda/k}. \quad (101)$$

Using this we may recast the system consisting of (91)_{1,2}, (96), (98) and (99) in the non-dimensional form

$$\dot{x}(t) = \cos \psi, \quad \dot{y}(t) = \sin \psi, \quad x\dot{\psi} = 2xh - \sin \psi, \quad l = x\dot{h} \quad (102)$$

and

$$\dot{l} = x[h - 2h(h - x^{-1} \sin \psi)^2], \quad (103)$$

where

$$t = \mu s, \quad x = \mu r, \quad y = \mu z, \quad h = H/\mu, \quad l = L/\mu \quad (104)$$

and $(\cdot)' = d(\cdot)/dt$. The boundary conditions (100) become

$$x(0) = \mu a, \quad \dot{h}(0) = \frac{1}{2}\sigma/\lambda, \quad \psi(0) = 0, \quad y(0) = 0 \quad (105)$$

and $h(T) = 0$, where $T = \mu S$. Typical data (see [18]) indicate that μ^{-1} is approximately an order of magnitude larger than the bilayer thickness. Thus, if μa is on the order of 1/10, say, then the cylinder radius is comparable to the thickness. This is appropriate if the cylinder represents a transmembrane protein [2]. Numerical solutions, obtained using Matlab ('bvp4c'), are discussed and compared to the predictions of a linear model in Sect. 5.

As a check on the solution, we use it to evaluate the energies (modulo 2π)

$$E_H(T) = \int_0^S H^2 r ds = \int_0^T h^2 x dt \quad \text{and} \quad E_K(T) = \int_0^S K r ds = \int_0^T x^{-1} \dot{\psi} (\sin \psi) x dt = 1 - \cos \psi(T) \quad (106)$$

associated with the mean and Gaussian curvatures, respectively. The total energy in the region $[0, T]$ is (cf. (26)) $E(T) = 2\pi[kE_H(T) + \bar{k}E_K(T)]$, and the solution is meaningful only if this converges to a finite value as T increases indefinitely. This is borne out by the computations, performed, for purposes of illustration, with $\mu a = 0.1$ and $\sigma/\lambda = -15$ (Fig. 4).

Fig. 4 Convergence of energy to a finite value

5 Linear theory in the Monge representation

In some circumstances it is appropriate and convenient to use the Monge representation

$$\mathbf{r}(\theta^\alpha) = \boldsymbol{\theta} + z(\boldsymbol{\theta})\mathbf{k} \quad (107)$$

of ω , where $\boldsymbol{\theta}$ is position on a plane p with unit normal $\mathbf{k}$. The shape of the membrane is then determined by the single function $z(\boldsymbol{\theta})$. For example, p may be parametrized globally by a single system of Cartesian coordinates θ^α , in which case

$$\boldsymbol{\theta} = \theta^\alpha \mathbf{e}_\alpha, \quad (108)$$

where $\{\mathbf{e}_\alpha\}$ is an orthonormal basis for the plane. These then furnish a parametrization of ω via (107). We compute

$$\mathbf{a}_\alpha = \mathbf{e}_\alpha + z_{,\alpha}\mathbf{k}, \quad a_{\alpha\beta} = \delta_{\alpha\beta} + z_{,\alpha}z_{,\beta} \quad \text{and} \quad \mathbf{n} = (\mathbf{k} - \nabla_p z)/\sqrt{a}, \quad (109)$$

where $\delta_{\alpha\beta}$ is the Kronecker delta, $\nabla_p z = z_{,\alpha}\mathbf{e}_\alpha$ is the gradient on p , and

$$a = \det(a_{\alpha\beta}) = 1 + |\nabla_p z|^2. \quad (110)$$

Further,

$$b_{\alpha\beta} = \mathbf{n} \cdot \mathbf{a}_{\alpha,\beta} = z_{,\alpha\beta}/\sqrt{a}, \quad (111)$$

and the curvature tensor is $\mathbf{b} = b_{\alpha\beta}\mathbf{a}^\alpha \otimes \mathbf{a}^\beta$, where

$$\mathbf{a}^1 = \frac{1}{a} \{ [1 + (z_{,2})^2](\mathbf{e}_1 + z_{,1}\mathbf{k}) - z_{,1}z_{,2}(\mathbf{e}_2 + z_{,2}\mathbf{k}) \}, \quad (112)$$

together with a similar formula for $\mathbf{a}^2$, obtained by interchanging $z_{,1}$ and $z_{,2}$. These are derived by using $\mathbf{a}^\alpha = a^{\alpha\beta}\mathbf{a}_\beta$, with $(a^{\alpha\beta}) = (a_{\alpha\beta})^{-1}$.

5.1 Linearization

We obtain the linear theory for the case in which the gradients of $z(\boldsymbol{\theta})$ of all orders are small, so that their products can be neglected. Using the notation $\simeq$ to identify equations valid to linear order, we then have

$$a \simeq 1, \quad \mathbf{n} \simeq \mathbf{k} - \nabla_p z, \quad \mathbf{a}^\alpha \simeq \mathbf{e}_\alpha + z_{,\alpha} \mathbf{k} \quad \text{and} \quad \mathbf{b} \simeq \nabla_p^2 z, \quad (113)$$

where $\nabla_p^2 z = z_{,\alpha\beta} \mathbf{e}_\alpha \otimes \mathbf{e}_\beta$ is the second gradient on p . The mean and Gaussian curvatures are given by

$$H \simeq \frac{1}{2} \Delta_p z \quad \text{and} \quad K \simeq 0, \quad (114)$$

where $\Delta_p z = \text{tr}(\nabla_p^2 z)$ is the Laplacian on p .

The foregoing approximations yield the linearization of the shape equation (27) for uniform Helfrich membranes. For the case of vanishing pressure, this is

$$\frac{1}{2} k \Delta_p (\Delta_p z) - \lambda \Delta_p z \simeq 0, \quad (115)$$

where λ is constant in accordance with (16).

Let $\bar{\mathbf{r}}(S) = \mathbf{r}(\bar{\boldsymbol{\theta}}(S))$, where $\bar{\boldsymbol{\theta}}(S)$ is the arclength parametrization of the projection of the curve $\partial\omega$ on the plane p . We have

$$\bar{\mathbf{r}}'(S) = \boldsymbol{\tau}_p + (\boldsymbol{\tau}_p \cdot \nabla_p z) \mathbf{k}, \quad \text{where} \quad \boldsymbol{\tau}_p = \bar{\boldsymbol{\theta}}'(S) \quad (116)$$

is the unit tangent to the projected curve. Then, (32) furnishes

$$\bar{\mathbf{r}}'(S) = |\bar{\mathbf{r}}'(S)| \boldsymbol{\tau}, \quad \text{where} \quad |\bar{\mathbf{r}}'(S)| = \sqrt{1 + (\boldsymbol{\tau}_p \cdot \nabla_p z)^2}. \quad (117)$$

Accordingly,

$$\boldsymbol{\tau} \simeq \boldsymbol{\tau}_p + (\boldsymbol{\tau}_p \cdot \nabla_p z) \mathbf{k}, \quad (118)$$

and (113)₂ yields

$$\mathbf{v} = \boldsymbol{\tau} \times \mathbf{n} \simeq \mathbf{v}_p + \nabla_p z \times \boldsymbol{\tau}_p, \quad (119)$$

where $\mathbf{v}_p = \boldsymbol{\tau}_p \times \mathbf{k}$ is the unit normal to the projected curve. These in turn furnish

$$\mathbf{v} \times \boldsymbol{\tau} \simeq \mathbf{k} - [(\boldsymbol{\tau}_p \cdot \nabla_p z) \boldsymbol{\tau}_p + \boldsymbol{\tau}_p \times (\nabla_p z \times \boldsymbol{\tau}_p)] = \mathbf{k} - \nabla_p z \simeq \mathbf{n}, \quad (120)$$

as required. Further, (42) and (113)₄ yield

$$\kappa_v \simeq \mathbf{v}_p \cdot (\nabla_p^2 z) \mathbf{v}_p \quad \text{and} \quad \tau \simeq \boldsymbol{\tau}_p \cdot (\nabla_p^2 z) \mathbf{v}_p. \quad (121)$$

Then, from (52), (53) and (114) it follows that

$$M \simeq \frac{1}{2} k \Delta_p z + \bar{k} [\Delta_p z - \mathbf{v}_p \cdot (\nabla_p^2 z) \mathbf{v}_p], \quad F_\tau \simeq 0 \quad \text{and} \quad F_v \simeq \lambda. \quad (122)$$

The normal force is given in the exact theory by

$$F_n = \bar{k} \tau'(s) - k H_{,v}, \quad (123)$$

where $(\cdot)'$ and $(\cdot)_{,v}$ are the arclength and normal derivatives on $\partial\omega$. The first of these satisfies the estimate

$$\tau'(S) = \tau'(s) |\bar{\mathbf{r}}'(S)| \simeq \tau'(s), \quad (124)$$

where $\tau'(S) = \boldsymbol{\tau}_p \cdot \nabla_p \tau$ is the arclength derivative on the projected curve. The second satisfies

$$H_{,v} = \mathbf{v} \cdot \mathbf{a}^\alpha H_{,\alpha} = (\mathbf{v}_p + \nabla_p z \times \mathbf{k} + \cdots) \cdot (\mathbf{e}_\alpha + z_{,\alpha} \mathbf{k} + \cdots) H_{,\alpha} \simeq \mathbf{v}_p \cdot \nabla_p H. \quad (125)$$

Accordingly,

$$F_n \simeq \bar{k} \boldsymbol{\tau}_p \cdot \nabla_p \tau - k \mathbf{v}_p \cdot \nabla_p H, \quad (126)$$

where τ and H are given by (121)₂ and (114)₁, respectively.

5.2 Solution

The result (122)₃ implies that λ is a (constant) isotropic stress in the surface ω . We solve (115) for the case $\lambda > 0$, corresponding to surface tension, regarded here as an assigned parameter; the case of surface pressure ($\lambda < 0$) is qualitatively different but can be treated in a similar manner. In this subsection we drop the subscript p from the notation for differential operators on the plane p and recast (115) as the Helmholtz equation

$$\Delta H - \mu^2 H = 0, \quad (127)$$

where μ is given by (101). The general solution, to be developed below, may then be used with (114)₁ to conclude that $\Delta z = 2H = (2/\mu^2)\Delta H$ and hence that $\Delta[z - (2/\mu^2)H] = 0$. This yields

$$z = (2/\mu^2)H + \varphi, \quad (128)$$

where φ is a plane harmonic function. Given the general solution to (127), this furnishes the integral $z(\theta)$ of the linearized shape equation. We note that the biharmonic shape equation $\Delta(\Delta z) = 0$, studied by Kim et al [2], corresponds to $\lambda = 0$. However, the general solution, which is well known [19], *cannot* be obtained from (128) simply by setting $\lambda = 0$. The present shape equation, with $\lambda > 0$, also arises in the strain-gradient theory of elasticity [20,21].

In polar coordinates (127) is

$$H_{,rr} + r^{-1}H_{,r} + r^{-2}H_{,\theta\theta} - \mu^2 H = 0. \quad (129)$$

Applying standard separation of variables and imposing periodicity in θ yields the azimuthal solutions $\cos m\theta$, $\sin m\theta$ with integer m , multiplied by functions of r that satisfy the modified Bessel equation of order m with parameter μ . The solutions are the modified Bessel functions of order m of the first and second kinds, denoted conventionally by $I_m(\mu r)$ and $K_m(\mu r)$, respectively [22]. These exhibit the asymptotic behavior $I_m(x) \sim \exp x/\sqrt{x}$ and $K_m(x) \sim \exp(-x)/\sqrt{x}$ at large x , modulo multiplicative constants. We seek a bounded solution on an unbounded domain $r \geq a(> 0)$ and thus conclude that

$$H(r, \theta) = \sum_{m=0}^{\infty} K_m(\mu r)(C_m \cos m\theta + D_m \sin m\theta), \quad (130)$$

where C_m and D_m are suitable constants. This yields $H^2 \sim \exp(-\alpha r)/r$ with α a positive constant, modulo a bounded multiplicative function of θ , which is integrable on the considered domain. Accordingly, the associated contribution to the net bending energy is finite.

Regarding φ , the periodic harmonic functions of r and θ are

$$(r/a)^n \cos n\theta, \quad (r/a)^n \sin n\theta, \quad (a/r)^n \cos n\theta, \quad (a/r)^n \sin n\theta; \quad n = 1, 2, 3, \dots, \quad \text{and} \quad \log(r/a). \quad (131)$$

We impose the requirement $|\nabla z| \rightarrow 0$ for large r to ensure that $\mathbf{n} \rightarrow \mathbf{k}$. This entails $z_{,r} \rightarrow 0$ and $r^{-1}z_{,\theta} \rightarrow 0$ and thus implies that

$$\begin{aligned} z(r, \theta) = & A + B \log(r/a) + (2C_0/\mu^2)K_0(\mu r) \\ & + \sum_{n=1}^{\infty} \{ [A_n(a/r)^n + (2C_n/\mu^2)K_n(\mu r)] \cos n\theta \\ & + [B_n(a/r)^n + (2D_n/\mu^2)K_n(\mu r)] \sin n\theta \}. \end{aligned} \quad (132)$$

From (113)₄,

$$\mathbf{b} \simeq z_{,rr}\mathbf{e}_r \otimes \mathbf{e}_r + r^{-2}(rz_{,r} + z_{,\theta\theta})\mathbf{e}_\theta \otimes \mathbf{e}_\theta + r^{-1}(z_{,r\theta} - r^{-1}z_{,\theta}) (\mathbf{e}_r \otimes \mathbf{e}_\theta + \mathbf{e}_\theta \otimes \mathbf{e}_r). \quad (133)$$

Therefore, $|\mathbf{b}| \sim r^{-2}$ and $|K| \sim r^{-4}$. The latter is integrable on the unbounded domain and this, together with the integrability of H^2 , implies that (132) furnishes the general finite-energy solution.

We use this solution to solve the linear version of the problem considered in Sect. 4.4. Thus we seek an axisymmetric solution for which all θ -derivatives of z vanish. Accordingly,

$$z(r) = A + B \log(r/a) + (2C_0/\mu^2)K_0(\mu r). \quad (134)$$

The boundary condition (86)₁, namely $F_n = \sigma$, reduces to $H'(a) = \sigma/k$, where $H(r) = C_0 K_0(\mu r)$. The condition $\gamma = \pi/2$; i.e., $\mathbf{n} = \mathbf{k}$ at $r = a$, reduces to $z'(a) = 0$. We also impose $z(a) = 0$ to facilitate comparison with the nonlinear solution, obtaining

$$z(r) = \frac{2\sigma}{k\mu^3 K'_0(\mu a)} [K_0(\mu r) - K_0(\mu a)] - \frac{a\sigma}{\lambda} \log(r/a). \quad (135)$$

The linear theory predicts that z and its derivatives are proportional to σ , and so we expect the linear solution to be valid if $|\sigma/\lambda|$ is sufficiently small. This expectation is supported by solutions to the nonlinear model of Sect. 4.4, depicted in Fig. 5 for $\mu a = 0.1$. These are seen to agree with the linear solution at smaller values of the hydrophobicity $|\sigma/\lambda|$, while larger values induce a significant depression in the membrane and consequent nonlinearity in the response. The cylinder generates a net vertical force $F = 2\pi a\sigma$ which approximates a downward point load on the membrane if the cylinder radius a is sufficiently small compared to the natural length scale μ^{-1} . Point loads are discussed in detail in Sect. 6.2. The effect of increasing the cylinder radius at fixed hydrophobicity is to increase the disparity between the linear and nonlinear solutions. This is due to the increase in the net force applied to the membrane, and is illustrated in Fig. 6 in the case of hydrophobicity $|\sigma/\lambda| = 1$.

Fig. 5 Solution of the conical anchoring problem with $\gamma = \pi/2$. Nonlinear solution (solid line); linear solution (dashed line): **a** $\sigma/\lambda = -3$, **b** $\sigma/\lambda = -9$, **c** $\sigma/\lambda = -15$

Fig. 6 Effect of cylinder radius: **a** $\mu a = 0.1$, **b** $\mu a = 10.0$

6 Adhesion

The results of Sects. 3 and 4 are used here to analyze the adhesion of a lipid membrane to a rigid substrate Γ with orientation $\mathbf{N}$. This setting furnishes a model for the adhesion of cell biomembranes [23–30]. Let the membrane be in contact with the substrate over the region $\omega_c \subset \Gamma$, and let $\omega_f = \omega \setminus \omega_c$ be the free part of the membrane. This problem differs from that considered in the foregoing in that contact does not occur at an edge of the membrane but rather over a portion of its interior. Let p be the common boundary of ω_c and ω_f (Fig. 7).

We consider a parametrized family of configurations that maintain contact with Γ . For these tangential variations of the membrane position are admissible in ω_c , while arbitrary variations are admissible in the interior of ω_f . Stationarity of the energy thus implies that (16) is valid in each of ω_c and ω_f separately. Henceforth we consider the membrane to be uniform in the sense that W does not depend explicitly on the coordinates θ^α . It follows from (16) that

$$\lambda = \lambda_c \text{ in } \omega_c \text{ and } \lambda = \lambda_f \text{ in } \omega_f, \quad (136)$$

respectively, where λ_c and λ_f are constants. Further, the shape equation (23) remains valid in ω_f with $\lambda = \lambda_f$. We assume the membrane to be closed (Fig. 7) and inflated by a uniform osmotic pressure of prescribed intensity. Thus the volume of liquid enclosed by the membrane is not prescribed. This models cell–substrate interactions over time scales sufficient for osmosis to be operative [23]. The considerations of Sect. 3 leading to (23) remain valid in this case, but with P interpreted as an assigned constant rather than a Lagrange multiplier.

6.1 Jump condition

The procedure described in Sect. 4 may be used to derive conditions that apply on the perimeter p of the contact region. Thus, let $\mathbf{v}_c$ be the exterior unit normal to ω_c on p , and let $\boldsymbol{\tau}_c = \mathbf{n} \times \mathbf{v}_c$. To prevent unbounded bending energy, we take the normal $\mathbf{n}$ to the membrane to be continuous everywhere on ω and hence on p . Then, $\mathbf{v}_f = -\mathbf{v}_c$ and $\boldsymbol{\tau}_f = -\boldsymbol{\tau}_c$ are the normal and tangent to $\partial\omega_f$. The subsurfaces ω_c and ω_f each contribute a boundary working term of the form (51). Taking $\mathbf{u} \in T_\Gamma$ on p , adding the two contributions and incorporating the variation (62) of the adhesion energy (with $\Gamma^* = \omega_c$ and $\mathbf{t} = \mathbf{v}_c$), we derive the residual working

$$\dot{E}_p = \int_p (P_v \mathbf{v}_c + P_\tau \boldsymbol{\tau}_c) \cdot \mathbf{u} ds, \quad (137)$$

where

$$P_v = [F_v] - [M] \mathbf{v}_c \cdot \mathbf{B} \mathbf{v}_c - \sigma \text{ and } P_\tau = [F_\tau] - [M] \boldsymbol{\tau}_c \cdot \mathbf{B} \boldsymbol{\tau}_c. \quad (138)$$

Here we use the notation defined by $[\cdot] = (\cdot)_c - (\cdot)_f$, where the subscripts c and f refer to the limits as p is approached from the contacting and free parts of the membrane, respectively. Further, we have assumed p to be a smooth curve, the substrate to have a continuous curvature tensor $\mathbf{B}$, and combined (47), (48) and (83) with

Fig. 7 Vesicle adhering to a rigid substrate

$\mathbf{n} = -\mathbf{N}$ (Fig. 7) on the closure of ω_c to obtain $\boldsymbol{\tau} \cdot \boldsymbol{\omega} = \mathbf{u} \cdot \mathbf{B}\mathbf{v}$ on $\partial\omega_c = \partial\omega_f (= p)$, with $\{\boldsymbol{\tau}, \mathbf{v}\} = \{\boldsymbol{\tau}_c, \mathbf{v}_c\}$ or $\{\boldsymbol{\tau}_f, \mathbf{v}_f\}$ as appropriate. Evidently adhesion furnishes an example of both hard and conical anchoring, the latter with $\gamma = \pi$ (cf. (80)). We note that contact is promoted ($\sigma > 0$) if the wall is hydrophilic, as it then exhibits affinity for the hydrophilic head groups of the lipid bilayer.

For $\mathbf{u} \cdot \mathbf{v}_c = 0$ on p the stationary-energy condition reduces to $\int_p P_\tau \boldsymbol{\tau}_c \cdot \mathbf{u} ds = 0$, and since this holds for all such $\mathbf{u}$ we require that $P_\tau = 0$ on p . The contribution of the constant Lagrange multipliers λ_c and λ_f to the residual stationary-energy condition is seen, with reference to (53) and (138), to reduce to $[\lambda] \int_p \mathbf{u} \cdot \mathbf{v}_c ds$. We consider divergence-free tangential variations $\mathbf{u}$ on ω_c . These satisfy

$$\int_p \mathbf{u} \cdot \mathbf{v}_c ds = 0 \quad (139)$$

and reduce the residual energy variation (64) to

$$\dot{E}_p = \int_p Q_v \mathbf{v}_c \cdot \mathbf{u} ds, \quad (140)$$

where

$$Q_v = [W - \kappa_v M] - [M] \mathbf{v}_c \cdot \mathbf{B}\mathbf{v}_c - \sigma. \quad (141)$$

Let $\mathbf{u} \cdot \mathbf{v}_c = G(s)$ on p , where G satisfies $\int_p G ds = 0$ but is otherwise arbitrary. This ensures that (139) is satisfied and yields the necessary condition $\int_p G Q_v ds = 0$ for stationarity of the energy, so that Q_v is orthogonal to all G meeting the stated restriction. The smooth curve p is diffeomorphic to a circle. The orthogonality condition then implies that all Fourier coefficients of Q_v vanish, so that Q_v vanishes almost everywhere on p . Altogether, we have the jump conditions

$$[F_\tau] - [M] \boldsymbol{\tau}_c \cdot \mathbf{B}\mathbf{v}_c = 0 \quad \text{and} \quad [W - \kappa_v M] - [M] \mathbf{v}_c \cdot \mathbf{B}\mathbf{v}_c = \sigma \quad \text{on } p. \quad (142)$$

We suppose the parametrization $\mathbf{r}(\theta^\alpha)$ of ω to be piecewise C^2 with discontinuities in the second derivatives, if any, occurring on p . These are of the form [10, 31] $[\mathbf{r}_{,\alpha\beta}] = \mathbf{a} v_\alpha v_\beta$ for some three-vector $\mathbf{a}$, yielding $[\mathbf{b}] = (\mathbf{a} \cdot \mathbf{n}) \mathbf{v} \otimes \mathbf{v}$. It follows from this and (42) that $\mathbf{a} \cdot \mathbf{n} = [\kappa_v]$ and $[\kappa_\tau] = [\tau] = 0$. Using these results with (53)₂ and $[fg] = [f]\langle g \rangle + \langle f \rangle[g]$, where $\langle \cdot \rangle$ is the average of the limits of the enclosed quantity from ω_c and ω_f , we reduce (142)₁ to

$$[M](\langle \tau \rangle + \boldsymbol{\tau}_c \cdot \mathbf{B}\mathbf{v}_c) = 0. \quad (143)$$

Because $\mathbf{n} = -\mathbf{N}$ on the closure of ω_c , we have $\mathbf{B} = -\mathbf{b}_c$ thereon, and thus $\langle \tau \rangle + \boldsymbol{\tau}_c \cdot \mathbf{B}\mathbf{v}_c = -\frac{1}{2}[\tau] (= 0)$, so that (143) is identically satisfied. In the same way (142)₂ may be written

$$[W] - [M](\langle \kappa_v \rangle + \mathbf{v}_c \cdot \mathbf{B}\mathbf{v}_c) - \langle M \rangle [\kappa_v] = \sigma, \quad (144)$$

where $\langle \kappa_v \rangle + \mathbf{v}_c \cdot \mathbf{B}\mathbf{v}_c = -\frac{1}{2}[\kappa_v]$. This and $\frac{1}{2}[M] - \langle M \rangle = -M_f$ furnish the single non-trivial jump condition

$$[W] - M_f [\kappa_v] = \sigma, \quad (145)$$

which generalizes that derived by Rosso and Virga [3, eq. (4.13)] for surfaces of revolution.

For the Helfrich energy defined by (26), we use (52) and (145) to obtain

$$[W] = \frac{1}{4}k[\kappa_v^2] + \left(\frac{1}{2}k + \bar{k}\right)\kappa_\tau[\kappa_v], \quad M_f = \frac{1}{2}k\{(\kappa_v)_f + \kappa_\tau\} + \bar{k}\kappa_\tau \quad \text{and} \quad \sigma = \frac{1}{4}k\{[\kappa_v^2] - 2\kappa_v_f\}. \quad (146)$$

Finally,

$$\sigma/k = \frac{1}{4}[\kappa_v]^2 = [H]^2, \quad (147)$$

in agreement with Eq. (4.14) of Rosso and Virga [3] (see also [4, 23]). This condition implies that finite-area adhesive contact with a hydrophobic wall ($\sigma < 0$) is impossible. Further, we note that for membranes of the Helfrich type, curvature discontinuities in the interior of the free part of the membrane are precluded by certain phase-equilibrium conditions derived in [10].

6.2 Point loads

We are interested in the response of the adhering membrane to a point load exerted on ω_f . The point load simulates the force generated by the tip of an AFM probe [32,33]. Here, we suppose the membrane to be a surface of revolution acted upon by a vertically-directed force F applied at its north pole. If the load is dead, we may model it by subtracting the term Fz_p from the expression for the total energy, where z_p is the current z -coordinate of the point where the load is applied [13,34,35]. A natural boundary condition involving F then follows from the stationarity of the energy with respect to variations $\dot{z}_p$. If such variations are precluded; i.e., if z_p is assigned, then F is to be regarded as a reaction force required to maintain the assigned value. In this case there is no adjustment to the expression for the total energy.

Alternatively, and equivalently, the desired boundary condition follows from the equilibrium of a sub-surface $\tilde{\omega} \subset \omega_f$ containing the pole, bounded by a parallel of latitude defined by $s = \tilde{s}$, where s measures arclength along the meridian from the pole where the load is applied. This is expressed by

$$\int_{\tilde{\omega}} P \mathbf{n} da + \int_{\partial \tilde{\omega}} \mathbf{f} dt + F \mathbf{k} = \mathbf{0}, \quad (148)$$

where $t = r(\tilde{s})\theta$ measures arclength around the perimeter of the parallel, $\mathbf{f}$ is the force per unit length exerted on $\tilde{\omega}$ by the part $\omega \setminus \tilde{\omega}$ of the membrane, and $\mathbf{k}$ is the direction of the point load along the axis of symmetry (see Sect. 4.3). Because parallels of latitude are lines of curvature on the membrane, τ vanishes on $\partial \tilde{\omega}$ and (cf. (51))

$$\mathbf{f} = F_v \tilde{\mathbf{v}} + F_n \mathbf{n}, \quad (149)$$

where $\tilde{\mathbf{v}}$ is the exterior unit normal to $\tilde{\omega}$ (the opposite of $\mathbf{v}$ in (92)₁), $\mathbf{n}$ is given by (92)₃, and (cf. (53))

$$F_v = W + \lambda - \kappa_v M, \quad F_n = -\frac{1}{2}(W_H)' - \kappa_\tau (W_K)', \quad (150)$$

where $(\cdot)' = d(\cdot)/ds$. Thus,

$$\mathbf{f} = (F_v \cos \psi - F_n \sin \psi) \mathbf{e}_r + (F_v \sin \psi + F_n \cos \psi) \mathbf{k}. \quad (151)$$

The periodicity of $\mathbf{e}_r(\theta)$ then yields

$$\int_{\partial \tilde{\omega}} \mathbf{f} dt = 2\pi r(\tilde{s})(F_v \sin \psi + F_n \cos \psi) \mathbf{k}. \quad (152)$$

The boundedness of the assigned osmotic pressure P , together with (148) and the conditions

$$r(0) = 0, \quad \psi(0) = 0 \quad (153)$$

at the point of load application, delivers

$$F/2\pi = -\lim_{\tilde{s} \rightarrow 0} (r F_n). \quad (154)$$

For the Helfrich energy this reduces to

$$F/2\pi = k \lim_{\tilde{s} \rightarrow 0} (r H'), \quad \text{yielding } L(0) = F/2\pi k, \quad (155)$$

where $L(s)$ is defined by (99). The system (91)_{1,2}, (96), (98), (99) furnishes the relevant differential equations in this case. In view of (153)₁, these contain a singularity at $s = 0$. To treat this numerically, we assign data at a very small value of s instead, denoted here and henceforth by $s = 0^+$. The relevant data are obtained by deriving the asymptotic structure of the solution for s near zero. For example, (91)₁, (99) and (155)₂ yield $r(s) \sim s$ and $s H'(s) \sim L(s) \sim F/2\pi k$. Then, $H(s) \sim (F/2\pi k) \log s + C$, where C is a constant. Equation (96), which may be written in the form $d(r \sin \psi)/dr = 2rH$, then combines with (153)₂ to give $\sin \psi \sim (F/2\pi k)s \log s + (C/2)s$. Accordingly we assign

$$r(0^+) = 0, \quad \psi(0^+) = 0 \quad \text{and} \quad L(0^+) = F/2\pi k. \quad (156)$$

The surface area of a sector $[0, s]$ of the membrane is

$$a(s) = 2\pi \int_0^s r(t) dt. \quad (157)$$

We have $a'(s) = 2\pi r(s) (> 0)$, implying that a and s are in one-to-one correspondence and hence that the former may be used in place of the latter as independent variable. The constraint on surface area is then enforced simply by integrating the equations over the domain $[0, A]$, where A is the assigned membrane area. For the Helfrich energy, the relevant differential equations, holding on the free part of the membrane, are (cf. (91)_{1,2}, (96), (98), (99))

$$2\pi r r'(a) = \cos \psi, \quad 2\pi r z'(a) = \sin \psi, \quad 2\pi r^2 \psi'(a) = 2rH - \sin \psi \quad (158)$$

and

$$2\pi L'(a) = (2\lambda/k)H - 2H(H - r^{-1} \sin \psi)^2, \quad \text{where } L = 2\pi r^2 H'(a). \quad (159)$$

We have assigned nil osmotic pressure ($P = 0$) and set $\lambda_f = \lambda$. The force boundary condition (156)₃ remains unchanged. These equations apply on the domain $[0, A_f]$, where $A_f = A - A_c$ is the surface area of the free membrane and A_c is the surface area of the part in contact with the substrate.

Typically, the point load F is part of the assigned data. However, this is not convenient from the viewpoint of numerical analysis. Instead, we adopt a procedure similar to that used in [36]. Thus, given A we assign $A_f \in (0, A)$ and compute the solution numerically subject to the boundary conditions

$$r(0^+) = 0, \quad \psi(0^+) = 0, \quad r(A_f) = r_p, \quad z(A_f) = z_p \quad \text{and} \quad \psi(A_f) = \psi_p, \quad (160)$$

together with (156) and (147), the latter giving the value of H in the free membrane, at the curve p separating it from the part in contact; i.e., at $a = A_f$. Further, r_p , z_p and ψ_p are known from the geometry of the substrate. Altogether, these furnish data sufficient to solve for r , z , ψ , H , L , the parameter λ , and the force F .

To non-dimensionalize this system, we note that a complete sphere ($H = \text{const.}$) furnishes an equilibrium shape, provided that A_c , F and λ all vanish. This follows easily from (27), with $K = H^2$. The radius of this sphere, R say, furnishes a length scale, which we use to define the dimensionless variables

$$\alpha = a/(2\pi R^2), \quad x = r/R, \quad y = z/R, \quad h = RH, \quad l = RL \quad \text{and} \quad \bar{\lambda} = R^2 \lambda/k. \quad (161)$$

In term of these the differential equations are

$$x\dot{x} = \cos \psi, \quad x\dot{z} = \sin \psi, \quad x^2\dot{\psi} = 2xh - \sin \psi, \quad x^2\dot{h} = l \quad (162)$$

and

$$\dot{l} = 2h[\bar{\lambda} - (h - x^{-1} \sin \psi)^2], \quad (163)$$

where $(\cdot)' = d(\cdot)/d\alpha$, and the boundary conditions are

$$x(0^+) = 0, \quad \psi(0^+) = 0, \quad x(\alpha_f) = x_p, \quad y(\alpha_f) = y_p \quad \text{and} \quad \psi(\alpha_f) = \psi_p, \quad (164)$$

together with

$$[h]^2 = \bar{\sigma} \quad \text{and} \quad l(0^+) = \bar{F}, \quad (165)$$

where

$$\bar{\sigma} = R^2 \sigma/k \quad \text{and} \quad \bar{F} = FR/(2\pi k). \quad (166)$$

The total area is constrained to be that of the spherical membrane, namely $4\pi R^2$. Accordingly, the equations are integrated over the domain $[0, \alpha_f]$ with an assigned value of $\alpha_f \in (0, 2)$. For Helfrich membranes the shapes obtained are universal in the sense that they are not affected by the bending modulus k .

Numerical simulations, obtained with $\bar{\sigma} = 4$, are shown in Figs. 8, 10, and 12. These depict the shapes of membranes interacting with substrates that are either flat or uniformly curved. In each case the dashed contour represents the meridian of the membrane corresponding to vanishing point load. The solid curves correspond

Fig. 8 Equilibrium shapes of a vesicle adhering to a flat substrate ($\bar{\sigma} = 4$). Dashed curve corresponds to vanishing point load

Fig. 9 Pole force versus contact area for a vesicle adhering to a flat substrate ($\bar{\sigma} = 4$)

to membranes under compressive (downward) or tensile (upward) point loads. Also shown, in Figs. 9, 11, and 13, are the pole forces as functions of contact area. These exhibit maxima at intermediate values of area corresponding to tensile point loads. Accordingly, the contact area associated with an assigned point load is non-unique over some interval of tensile load. For assigned loads in this interval, we have evaluated the total system energy consisting of the membrane bending energy, adhesion energy and the load potential. In each case the energy associated with the larger contact area was found to be lower than that of the smaller-area alternative. Given that no equilibria exist for point loads exceeding the computed maxima, we conclude that contact with the substrate is lost in a dynamic transition if the applied load is increased beyond the relevant maximum.

Also considered is a closed membrane with opposing point loads applied at its poles. Here we modify the conventional Helfrich energy to accommodate a *spontaneous curvature* C . Thus, in place of (26) we use [12]

$$W = k(H - C)^2 + \bar{k}K, \quad (167)$$

in which the term involving K may be suppressed if the genus of the surface is invariant. This is a well known consequence of the Gauss–Bonnet theorem. We take C to be an assigned constant. The associated shape equation, replacing (163), is easily derived (e.g., [6]) and found to be

$$\dot{l} = 2h[(h - c)^2 + \bar{\lambda}] - 2(h - c)(h - x^{-1} \sin \psi)^2, \quad (168)$$

Fig. 10 Equilibrium shapes of a vesicle adhering to a concave substrate ($\bar{\sigma} = 4$). Dashed curve corresponds to vanishing point load

Fig. 11 Pole force versus contact area for a vesicle adhering to a concave substrate ($\bar{\sigma} = 4$)

Fig. 12 Equilibrium shapes of a vesicle adhering to a convex substrate ($\bar{\sigma} = 4$). Dashed curve corresponds to vanishing point load

Fig. 13 Pole force versus contact area for a vesicle adhering to a convex substrate ($\bar{\sigma} = 4$)

Fig. 14 Naturally curved vesicle under tensile point loads at the poles

where

$$c = RC \quad (169)$$

is the dimensionless spontaneous curvature. Equations (162) are unaffected. A sphere of radius R (i.e., $H = -1/R$) furnishes a solution provided that $\lambda = 0$ and $C = H$. Accordingly, we set $c = -1$.

We assume the equator to be a plane of mirror symmetry and model the upper half of the surface only. Thus we integrate the equations on the domain $[0, 1]$. As argued in [10], mirror symmetry requires that the transverse shear force F_n vanish at the equator. From (53)₃, this implies that $H'(s) = 0$ at the appropriate value of arclength and hence that

$$\dot{h}(1) = 0. \quad (170)$$

The remaining boundary conditions are

$$x(0^+) = 0, \quad \psi(0^+) = 0, \quad \psi(1) = -\pi/2, \quad y(1) = 0, \quad \text{and} \quad l(0^+) = \bar{F}. \quad (171)$$

In practice we use the last of these to compute the point-load $\bar{F}$ required to maintain an assigned pole position $y_p = y(0^+)$.

Fig. 15 Force-deflection response of the naturally curved vesicle

Numerical simulations are displayed in Figs. 14 and 15. These indicate that the force required to maintain equilibrium is a non-monotone function of pole position, with a single maximum preceding a single minimum. Forces on the initial ascending portion of the curve are associated with three values of the pole position. Accordingly, the solution to the problem of assigned point load is non-unique for loads up to the local maximum value $\bar{F} \approx 0.275$. Calculations reveal that for every such value of force considered, the total energy associated with the initial ascending portion of the response curve is lower than those of the two alternative solutions. Our simulations thus support the conclusion that an actual membrane would *snap through* from the initial ascending portion of the curve to the second ascending portion at the local maximum value of the load. The pre- and post-snapped configurations correspond to the dashed contours in Fig. 14. The response upon further increase of the load is described by the second ascending branch. We have not encountered any global force maximum and thus conclude that equilibria exist over a wide, possibly unlimited, range of loads. The snap-through phenomenon may be understood via an analogy with a naturally curved arch. The natural curvature of the arch is analogous to the spontaneous curvature of the membrane, corresponding to vanishing point load. As the membrane is pulled along the axis of symmetry by the load, it develops hoop stresses in its circles of latitude. These play the role of a distributed transverse load in the analogous arch problem, which acts to promote the snap-through effect.

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