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VARIATIONAL AND FINITE ELEMENT ANALYSIS OF VIBROEQUILIBRIA[1]

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Abstract — We adapt, via asymptotic expansion, Kapitsa's formula for the effective potential of a pendulum with vibrating suspension to rapidly forced potential flows with free boundaries. Determination of time-averaged stationary states leads to an optimal shape design problem. Under periodic boundary conditions existence and uniqueness of smooth minimizers to the averaged energy is proved using local coerciveness. In the numerical part of the article, 2D and 3D finite element approximations including related error estimates are discussed. Some illustrating examples are sketched.

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Introduction

This paper concerns the averaging of rapidly forced systems applied to free boundary potential flows in a gravity field. The investigation of liquids subject to vibrations has a long history starting with the famous Faraday experiments [1, 7] which show, e.g. the generation of capillary waves along the surface of a liquid in a vertically vibrating container. Here we are interested in phenomena resulting from highly oscillating data after time averaging. This may be viewed as a kind of temporal homogenization as opposed to the homogenization of spatially periodic structures, cf. e.g. [6]. Seemingly Kapitsa [12] was the first to recognize that the upper position of a pendulum whose suspension is subjected to vertical oscillations, after raising frequency, eventually stabilizes. The general idea behind this type of averaging consists in decomposing the motion in a slow-time and a highly oscillating fast-time component. The observer essentially notices the slow-motion part. In various fields of physics and engineering averaging allows by rapidly forcing a given system, as in the case of the inverted pendulum, to stabilize originally unstable equilibria and create new equlibria as well.

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The Paul trap [16] exploits this principle to levitate charged particles via an oscillating electric field. An abundance of applications to finite dimensional mechanical devices can be found in the monograph [3]. For further related literature the reader is referred to the monographs [4, 14, 18] and to the recent paper [15] on the averaging of second-order differential equations and the references therein. The present text may be viewed as a continuation of our paper [2], with special emphasis on numerical viewpoints, but it can be read independently of that predecessor. We point further to [20] and to [9], the latter containing also references to experimental work on our subject.

In Section 1, we study systems the evolution of which is governed by an abstract nonlinear second-order differential equation and which are subjected to a high frequency excitation. Leaving aside questions concerning the well-posedness of the initial value problem, Proposition 1.1, via formal asymptotic expansion, characterizes the time-averaged solution path by an averaged differential equation. Averaging respects the variational structure. This is established in Proposition 1.2: relative to a conservative high-frequency disturbance averaging maintains the Euler-Lagrange character of a differential equation. In this case, the effective potential links to the original one via Legendre transformation.

Section 2 addresses averaging of incompressible potential flows with partially free boundaries in an oblique gravity field. Typically, the situation outlined here arises after relating a free boundary flow in a domain the boundary of which oscillates rapidly according to a given periodicity pattern relative to a fixed time-independent reference configuration. This includes, in the simplest situation, harmonic oscillations in a given space direction. Via transformation to a fixed reference domain we show smoothness of the effective potential within the class of Lipschitz domains. First and second derivatives of the potential are evaluated. The second derivative turns out to be semi-bounded in L^2.

In Section 3, assuming the data to be periodic and the gravity field sufficiently strong, we show the existence and uniqueness of smooth stationary states in the neighbourhood of a planar surface. This amounts to considering the free boundary condition as a nonlinear first-order elliptic pseudo-differential operator which depending on the data may be degenerated. This degeneration leads to a loss of differentiabilty in the linearized equation which forbids the application of the implicit function theorem. Instead, following Kato's proof of existence of periodic solutions for the first order PDE in [13], we solve the operator equation using a coerciveness argument. To show the smoothness of the solution, during the proof, some care must be taken in estimating the dependence of generic constants on the differentiability order. To maintain simplicity, we abstain from formulating our results under the weakest assumptions; some estimates may be considerably improved.

The finite element discretization of the optimal shape design problem considered above, in Section 4, runs essentially along usual lines, cf. [5, 10, 17]. Approximation of the free boundary by piecewise linear elements induces, via vertical interpolation, a subdivision of the flow domain. This allows to consider the heights of the nodes along the free boundary as the only variables to be dealt with. The computation of the discretized energy calls for the solution of a system of linear equations which results from the FEM formulation of a mixed boundary value problem for the Laplacian. Concerning the actual computation, it is advantageous that there is no need to solve an additional system to get the values of the discretized gradient. The main result of this Section consists in the proof of an error estimate for the discretized minimum problem which presupposes the existence of an exact solution with some degree of smoothness and the validity of a certain stability condition, cf. Theorem 4.3. The missing exponent one half in the error estimate reflects degeneracy of the pseudo-differential operator representing the free boundary condition.

In Section 5, for a few two- and three-dimensional examples, we collect some results of our numerical tests. Here we restrict ourselves to the determination of local minimizers. The algorithm is based on a successive line search in conjugate gradient directions. No attempt was made to determine the possibly existing equilibria which are merely critical points. Figs. 1–8 illustrate the interplay between the gravity and vibrational forces.

We conclude our introduction with a few remarks concerning the existence theory of the hydrodynamic equations considered here. Despite the considerable progress in the treatment of the Euler flow of an incompressible fluid within fixed boundaries, strong existence results remained less frequent as long as free boundaries are involved. A rigorous mathematical existence and uniqueness theory of flows with partially free boundaries, as considered here, due to the possible singularities at the edges, seems to be even more elusive.

1. Kapitsa averaging

This Section focuses on the averaging of rapidly forced systems modelled by ordinary as well as by partial differential equations. Whereas Proposition 1.1 describes the averaging of a second order equation, Proposion 1.2 is geared to a particular situation of variational equations. In the latter case the averaged equation is the Euler-Lagrange equation to a corresponding "averaged" Lagrangian whose potential energy part is referred to as the effective potential of the system.

Our exposition is based on formal asymptotic expansion. It presupposes differentiability to any order of the operators involved. In addition, we assume unique solvability of the initial value problem of the differential equations considered as well as for their homogenizations. This is guaranteed as far as ordinary differential equations and analytic data are concerned. Moreover, under this limitation, the asymptotic expansion below can be shown to be analytic in ε indeed. We abstain, however, from discussing this situation in detail since the equations of motion encountered in our hydrodynamical model are nonlinear PDEs.

We agree on some notation. In the following, a dot refers to differentiation in t. Capitals $F, G, \ldots$ are used for operators. $G'(\tau, u)u_1$ and $F'(u, v)(u_1, v_1)$ denote Gateaux derivatives in directions u_1 and (u_1, v_1) respectively. For any 2π-periodic function $f = f(\tau)$ we abbreviate the time averaging on $[0, 2\pi]$ by

$$\langle f\rangle = \frac{1}{2\pi}\int_0^{2\pi} f(\tau)\,d\tau.$$

In addition to the differentiation ∂_τ in τ, we introduce the left inverse ∂_τ^{-1} which sends a periodic function with average zero to a zero-average image.

Proposition 1.1. *Let $G = G(\tau, u)$ be 2π-periodic in τ with average $\big\langle G(., u)\big\rangle = 0$ for all u considered. Then the initial value problem $u(0) = \bar u_0$, $\dot u(0) = \bar u_1$ for the differential equation*

$$\ddot u = F(u, \dot u) + \varepsilon^{-1} G_\tau(\tau, u), \tag{1.1}$$

relative to a two-scale time t (to which the dot refers) and $\tau = t/\varepsilon$ respectively, has an asymptotic solution

$$u_\varepsilon(t) = u_0(t) + \varepsilon u_1(t, \tau) + \varepsilon^2 u_2(t, \tau) + \ldots, \tag{1.2}$$

where the coefficients u_n are 2π-periodic in the variable τ. The leading term u_0 is to be evaluated from the averaged equation

$$\ddot{u}_0 = \big\langle F\big(u_0, \dot{u}_0 + G(\tau, u_0)\big) - G'(\tau, u_0)\big\{G(\tau, u_0)\big\}\big\rangle. \tag{1.3}$$

The weakly varying parts $v_n(t) = \big\langle u_n(t, .)\big\rangle$ of the higher approximates are solutions of the linearization to (1.3) at u_0 and have to satisfy the related initial data, whereas their high-frequency parts are to be determined simply by quadratures in τ.

Proof. By (1.2), we have

$$\dot{u} = \dot{u}_0 + \varepsilon\left(\partial_t u_1 + \varepsilon^{-1}\partial_\tau u_1\right) + \ldots = u_0' + \varepsilon u_1' + \ldots$$

and

$$\ddot{u} = \ddot{u}_0 + \varepsilon\left(\partial_t^2 u_1 + 2\varepsilon^{-1}\partial_t\partial_\tau u_1 + \varepsilon^{-2}\partial_\tau^2 u_1\right) + \ldots = \varepsilon^{-1}\partial_\tau^2 u_1 + u_0'' + \varepsilon u_1'' + \ldots,$$

where the abbreviations

$$u_n' = \partial_t u_n + \partial_\tau u_{n+1}, \quad u_n'' = \partial_t^2 u_n + 2\partial_t\partial_\tau u_{n+1} + \partial_\tau^2 u_{n+2}$$

have been used. The above initial data require that the summands in (1.2) satisfy the initial conditions $u_0(0) = \bar{u}_0$, $u_0'(0,0) = \bar{u}_1$ and $u_n(0,0) = 0$, $u_n'(0,0) = 0$ for $n \geqslant 1$ respectively, which implies

$$\dot{u}_0 = \bar{u}_1 - \partial_\tau u_1, \quad \partial_t u_n = -\partial_\tau u_{n+1} \tag{1.4}$$

for their partial derivatives at $t = \tau = 0$.

Substituting (1.2) into the right-hand side operators, we get

$$F(u, \dot{u}) = \sum_{n\geqslant 0} \varepsilon^n F_n, \quad G_\tau(\tau, u) = \sum_{n\geqslant 0} \varepsilon^n G_n$$

in terms of formal expansions, where

$$F_0 = F(u_0, u_0'), \quad F_1 = F'(u_0, u_0')(u_1, u_1') \quad \text{etc.}$$

Inserting into the differential equation

$$\varepsilon^{-1}\partial_\tau^2 u_1 + u_0'' + \varepsilon u_1'' + \ldots = \varepsilon^{-1} G_0 + \sum_{n\geqslant 0} \varepsilon^n (F_n + G_{n+1})$$

and comparison of coefficients leads to the recurrence

$$\partial_\tau^2 u_1 = G_0 = G_\tau(\tau, u_0), \tag{1.5}$$
$$\partial_\tau^2 u_{n+1} = -\partial_t^2 u_{n-1} - 2\partial_t\partial_\tau u_n + F_{n-1} + G_n, \ n \geqslant 1. \tag{1.6}$$

The solution of (1.5) reads

$$u_1(t, \tau) = \partial_\tau^{-1} G(\tau, u_0) + v_1(t).$$

Here, for the time being, v_1 remains unknown. The same remark applies to initial values, which, due to (1.4), are to be chosen according to

$$\begin{aligned} u_1(0,0) &= \partial_\tau^{-1} G(\tau, \bar u_0)|_{\tau=0} + v_1(0) = 0, \\ \partial_t u_1(0,0) &= \partial_\tau^{-1} G'(\tau, \bar u_0)\big\{\bar u_1 - \partial_\tau u_1(0,0)\big\} + \dot v_1(0) = -\partial_\tau u_2(0,0), \end{aligned}$$

which means

$$\begin{aligned} v_1(0) &= \partial_\tau^{-1} G(\tau, \bar u_0)|_{\tau=0}, \\ \dot v_1(0) &= -\partial_\tau u_2(0,0) - \partial_\tau^{-1} G'(\tau, \bar u_0)\big\{\bar u_1 - \partial_\tau u_1(0,0)\big\}. \end{aligned} \tag{1.7}$$

To identify u_2, we have to refer to (1.6)

$$\partial_\tau^2 u_2 = -\partial_t^2 u_0 - 2\partial_t \partial_\tau u_1 + F_0 + G_1. \tag{1.8}$$

In the following we agree on the notation $v \sim 0$ if $\langle v \rangle = 0$. Obviously, we have $\partial_t \partial_\tau u_n \sim 0$, as well as

$$F_0 = F\big(u_0, \dot u_0 + G(\tau, u_0)\big) \sim \big\langle F\big(u_0, \dot u_0 + G(\tau, u_0)\big)\big\rangle,$$

and

$$G_1 = G'_\tau(\tau, u_0) u_1 \sim -G'(\tau, u_0)\partial_\tau u_1 \sim -\big\langle G'(\tau, u_0) G(\tau, u_0)\big\rangle.$$

Hence, (1.8) implies

$$\partial_\tau^2 u_2 \sim -\ddot u_0 + \big\langle F\big(u_0, \dot u_0 + G(\tau, u_0)\big) - G'(\tau, u_0) G(\tau, u_0)\big\rangle\,. \tag{1.9}$$

Observing $\partial_\tau^2 u_2 \sim 0$ to be the (necessary and sufficient) solvability condition for (1.8) relative to our solution class requires that the right-hand side of (1.9) vanishes, which establishes equation (1.3). The latter equation is subject to the initial conditions

$$u_0(0) = \bar u_0, \quad \dot u_0(0) = \bar u_1 - \partial_\tau u_1(0,0) = \bar u_1 - G(\tau, \bar u_0).$$

One should notice that in (1.8) v_1 is still an unknown function.

We proceed to identify u_3 and v_1, respectively

$$\partial_\tau^2 u_3 = -\partial_t^2 u_1 - 2\partial_t \partial_\tau u_2 + F_1 + G_2, \tag{1.10}$$

cf. (1.6). Clearly, $\partial_t^2 u_1 \sim \ddot v_1$, $2\partial_t \partial_\tau u_2 \sim 0$. At the same time, observing

$$\partial_\tau^2 u_2 = G'(\tau, u_0) v_1 + r$$

with the reminder r which depends only on u_0 and $\dot u_0$, we have

$$F_1 = F'(u_0, u_0')(u_1, u_1') \sim \big\langle F'\big(u_0, \dot u_0 + G(\tau, u_0)\big)\big(v_1, \dot v_1 + G'(\tau, u_0) v_1\big)\big\rangle + \bar r$$

and

$$\begin{aligned} G_2 &\sim -G'(\tau, u_0)\partial_\tau u_2 - G''(\tau, u_0)\{u_1, \partial_\tau u_1\} \\ &\sim -\big\langle G'(\tau, u_0)\{G'(\tau, u_0) v_1\} - G''(\tau, u_0)\{G(\tau, u_0), v_1\}\big\rangle + \bar s, \end{aligned}$$

where both remainders $\bar r$, $\bar s$ depend only on u_0 and $\dot u_0$ as well. Thus, using the abbreviation

$$\begin{aligned} L(u_0, \dot u_0)(v_1, \dot v_1) = {} & \big\langle F'\big(u_0, \dot u_0 + G(\tau, u_0)\big)\big(v_1, \dot v_1 + G'(\tau, u_0) v_1\big)\big\rangle \\ & - \big\langle G'(\tau, u_0)\{G'(\tau, u_0) v_1\} - G''(\tau, u_0)\{G(\tau, u_0), v_1\}\big\rangle, \end{aligned}$$

we are led to

$$\partial_\tau^2 u_3 \sim -\ddot{v}_1 + L(u_0, \dot{u}_0)(v_1, \dot{v}_1) + f_1,$$

$f_1 = \bar{r} + \bar{s}$. This shows the solvability condition for (1.10) to be

$$\ddot{v}_1 = L(u_0, \dot{u}_0)(v_1, \dot{v}_1) + f_1. \tag{1.11}$$

Obviously, the homogeneous part of (1.11) coincides with the linearization of the homogenized equation (1.3) at u_0.

As mentioned above, v_1 has to satisfy the initial conditions (1.7) which involve the derivative $\partial_\tau u_2(0,0)$. Although u_2 is unknown at the present stage its derivative $\partial_\tau u_2$ at the single point $t = \tau = 0$, in view of (1.8), may be calculated from the data known so far. This determines v_1 completely.

We continue inductively, assuming, for $n \geqslant 3$, knowledge of $u_0, \dots, u_{n-2}, \partial_\tau u_{n-1}$. Clearly, interest is to be directed to the compatibility conditions of (1.6)

$$\partial_\tau^2 u_{n+1} \sim -\ddot{v}_{n-1} + F_{n-1} + G_n. \tag{1.12}$$

Inspecting recurrence (1.6) leads to

$$\partial_\tau u_n = G'(\tau, u_0) v_{n-1} + r \tag{1.13}$$

with the remainder r depending on the known data only. Having (1.13) in mind, one finds

$$\begin{aligned} F_{n-1} &= F'(u_0, u_0')(v_{n-1}, \dot{v}_{n-1} + \partial_\tau u_n) + \bar{r} \\ &\sim \big\langle F'\big(u_0, \dot{u}_0 + G(\tau, u_0)\big)\big(v_{n-1}, \dot{v}_{n-1} + G'(\tau, u_0) v_{n-1}\big)\big\rangle + \bar{r} \end{aligned}$$

and

$$G_n \sim -\big\langle G'(\tau, u_0)\{G'(\tau, u_0) v_{n-1}\} + G''(\tau, u_0)\{G(\tau, u_0), v_{n-1}\}\big\rangle + \bar{s}$$

with the remainder terms $\bar{r}, \bar{s}$ which are known by the induction hypothesis. Inserting the last three relations into (1.12) shows that v_{n-1} satisfies the linearized equation (1.11), except for the value of f_1 which has to be suitably altered into f_{n-1}.

Referring to the initial values of v_{n-1}, it can be noted that knowlege, by the induction hypothesis, of the high-frequency part of u_{n-1} implies knowlegde of $v_{n-1}(0)$ via (1.4). At the same time, evaluation of $\dot{v}_{n-1}(0)$ requires additional information on the derivative $\partial_\tau u_n$ at $t = \tau = 0$. The latter value, however, may be taken from (1.13) remembering the induction hypothesis. Thus, v_{n-1} is completely determined. Finally, $\partial_\tau u_n$ has to be taken from (1.13). □

The particular case in which (1.1) is the Euler-Lagrange equation to the variational problem

$$\int_{t_0}^{t_1} L(\varepsilon, \tau, u, \dot{u})\, dt \to \min, \tag{1.14}$$

has a special interest. The following proposition shows that averaging maintains the variational structure.

Proposition 1.2. *Let*

$$L = T - U(u) - \varepsilon^{-1} V_\tau(\tau, u) \tag{1.15}$$

denote the Lagrangian of the variational integral (1.14)*. Assuming the kinetic energy T to depend quadratically on $\dot u$, we set $T(u, \dot u) = \frac{1}{2}\langle \Lambda(u)\dot u \,|\, \dot u\rangle$, where $\langle \cdot \,|\, \cdot \rangle$ denotes the pairing between some Banach space and its dual. Averaging the Euler equation of* (1.14) *then leads to the Euler equation of the averaged ("effective") Lagrangian*

$$\bar L = T - U(u) - \big\langle T^*\big(u, V'(\tau, u)\big)\big\rangle, \tag{1.16}$$

where T^* denotes the Legendre transform of T relative to $\dot u$ (the existence of which is tacidly presumed).

Proof. Relative to the pairing above the Euler equation of (1.15) reads

$$\ddot u = \Gamma - \Lambda(u)^{-1} U' - \varepsilon^{-1} \Lambda(u)^{-1} \partial_\tau V'$$

where

$$\Gamma(u)\dot u^2 = -\Lambda(u)^{-1}\Lambda'(u, \dot u)\dot u + \frac{1}{2}\Lambda(u)^{-1}\big\langle \Lambda(u)\dot u \,|\, \Lambda(u)^{-1}\Lambda'(u, .)\dot u\big\rangle$$

are the "Christoffel symbols". Consequently, we have

$$F(u, \dot u) = \Gamma(u)\dot u^2 - \Lambda(u)^{-1}U'(u), \quad G(\tau, u) = -\Lambda(u)^{-1}\partial_\tau V'(\tau, u)$$

in (1.1). According to (1.3) that data, after averaging, lead to

$$\ddot u = \Gamma - \Lambda^{-1}U' + \big\langle \Gamma\{\Lambda^{-1}V', \Lambda^{-1}V'\} - (\Lambda^{-1}V')'\{\Lambda^{-1}V'\}\big\rangle. \tag{1.17}$$

Remembering the relation

$$T^*(u, p) = \frac{1}{2}\big\langle p \,|\, \Lambda(u)^{-1}p\big\rangle, \tag{1.18}$$

the assertion follows after comparing the variational equation to (1.16) with (1.17). □

In the following section, in the hydrodynamic context, we concentrate on equilibrium states of the averaged system (1.16). By Proposition 1.2, this amounts for u_0 being a critical point

$$J'(u_0) = 0 \tag{1.19}$$

of the effective potential

$$J(u) = U(u) + \big\langle T^*\big(u, V'(\tau, u)\big)\big\rangle \tag{1.20}$$

of the system in question. Seen from the perspective of asymptotics (1.2) the equilibrium condition (1.19) expresses stationarity of its leading part only. It should be born in mind, however, that the higher order approximations, as before, contain slow-time components, which satisfy linear differential equations of the type

$$\ddot v + J''(u_0) = f_n \tag{1.21}$$

in the situation just considered, cf. (1.11). Disregarding the initial values and assuming the invertibility of $J''(u_0)$, we may also construct time-independent solutions of (1.21). In that case (1.2) simplifies to

$$u(t) = u_0 + \varepsilon u_1(\tau) + \varepsilon^2 u_1(\tau) + \dots,$$

where the dependency on t of the higher order terms drops out.

2. Averaging of free boundary flows

Here we zero in on a free boundary problem for potential flows in $\mathbb{R}^N$, $N \geqslant 2$. Let $x = (x_1, \dots, x_N)$ be Euclidian coordinates in $\mathbb{R}^N$, let $x' = (x_1, \dots, x_{N-1})$ and let t denote time. We consider the irrotatinal motion of perfect, incompressible fluid (with mass density $\rho = 1$) in a time-dependent domain

$$\Omega_u = \big\{x = (x', x_N) \in B \times \mathbb{R} \mid 0 < x_N < u(t, x')\big\},$$

which is part of a cylindrical container $B \times (0, \infty) \subset \mathbb{R}^N$. Its base $B \subset \mathbb{R}^{N-1}$ is assumed to be bounded with a Lipschitz continuous boundary ∂B. Let

$$\Sigma_u = \big\{x = (x', x_N) \in B \times \mathbb{R} \mid x_N = u(t, x')\big\}$$

be the free surface part of the total boundary Γ of Ω. In the following, if the meaning is clear, the subscript of Ω_u and Σ_u will be dropped. We presume the motion to be driven by the joint action of gravity in a constant direction $b \in \mathbb{R}^N$

$$U(u) = \int\limits_{\Omega} b \cdot x \, dx \tag{2.1}$$

and a velocity field which forces the bounding walls of the container to move as a rigid body with a spatially independent velocity $v = v(\tau)$. We assume v to be 2π-periodic in $\tau = t/\varepsilon$; $\varepsilon > 0$ denotes a small parameter. Then, relative to the reference system at rest, the corresponding action reads

$$A(\varepsilon, u) = \int\limits_{t_0}^{t_1} \left(\int\limits_{\Omega} \frac{1}{2} \big|\nabla\big(\varphi + v(\tau) \cdot x\big)\big|^2 \, dx - U \right) dt,$$

where the velocity potential φ of the flow has to satisfy Laplace's equation

$$\Delta\varphi = 0 \ \text{ in } \ \Omega$$

with Neumann data

$$\partial_n \varphi = \dot{u} \left(1 + |\nabla u|^2\right)^{-1/2} \ \text{ on } \ \Sigma, \qquad \partial_n \varphi = 0 \ \text{ on } \ \Gamma \setminus \Sigma. \tag{2.2}$$

Here ∂_n denotes the differentiation with respect to the outer normal. The volume conservation of the flow implies that the right-hand side of (2.2) being the normal component of the surface velocity has the mean value of zero. This assures the solvability condition for the Neumann problem to be met. By Green's formula and (2.2) we get

$$\int\limits_{\Omega} \nabla\varphi \nabla(v \cdot x) \, dx = \int\limits_{\Sigma} (v \cdot x) \, \partial_n \varphi \, do = \int\limits_{\Sigma} (v \cdot x) \, \dot{u} \, dx'$$

and, consequently,

$$\int\limits_{\Omega} \nabla\varphi \nabla\big(v \cdot x\big) \, dx = \frac{d}{dt} \int\limits_{B} \left(\sum_{i=1}^{N-1} v_i x_i u + \frac{1}{2} v_N u^2 \right) dx' - \frac{1}{\varepsilon} \int\limits_{\Omega} a(\tau) \cdot x \, dx$$

with $a(\tau) = dv(\tau)/d\tau$. Thus, neglecting the time derivatives, the action integral transforms into

$$A(\varepsilon, u) = \int_{t_0}^{t_1} \left(\int_\Omega \frac{1}{2} |\nabla \varphi|^2 \, dx - U - \varepsilon^{-1} V \right) dt,$$

where

$$V(\tau, u) = \int_\Omega a(\tau) \cdot x \, dx.$$

We keep the notations of Section 1. In the following, by constant vertical continuation, we identify the functions originally defined on Σ with functions having the domain of definition B. Introducing the solution ψ of

$$\Delta \psi = 0 \text{ in } \Omega,$$
$$\partial_n \psi = \dot{v} \left(1 + |\nabla u|^2\right)^{-1/2} \text{ on } \Sigma, \qquad \partial_n \psi = 0 \text{ on } \Gamma \setminus \Sigma,$$

we get by Green's formula

$$T(u)\{\dot{u}, \dot{v}\} = \frac{1}{2} \int_\Sigma \varphi \, \partial_n \psi \, do = \frac{1}{2} \int_\Sigma \dot{v} \left(C(u)^{-1} \dot{u} \right) dx'.$$

Here $C(u)$ denotes the map

$$f \mapsto C(u) f = (1 + |\nabla u|^2) \partial_n \chi|_\Sigma,$$

which sends the Dirichlet data f on Σ via the solution of the mixed BVP

$$\Delta \chi = 0 \text{ in } \Omega, \quad \chi|_\Sigma = f, \quad \partial_n \chi|_{\Gamma \setminus \Sigma} = 0, \tag{2.3}$$

(essentially) to normal derivatives. Hence, relating the boundary values on Σ to B, as agreed on above, we get

$$\Lambda(u) \dot{u} = C(u)^{-1} \dot{u},$$

and, accordingly,

$$T^*(u, p) = \frac{1}{2} \int_B p \, C(u) p \, dx'$$

in view of (1.18). Considering

$$V'(\tau, u) v = \int_\Sigma \big(a(\tau) \cdot x \big) \, v \, dx'$$

this implies

$$\left\langle T^\star \big(u, V'(\tau, u) \big) \right\rangle = \sum_{i,j=1}^N a_{ij} \int_\Sigma x_i \, C(u) x_j \, dx' \tag{2.4}$$

for the time average of $T^\star\big(u, V'(\tau, u)\big)$, where we have set

$$a_{ij} = \frac{1}{2} \big\langle a_i(\tau) a_j(\tau) \big\rangle = \frac{1}{4\pi} \int_0^{2\pi} a_i(\tau) a_j(\tau) \, d\tau.$$

Equality (2.4) simplifies to become

$$\big\langle T^\star\big(u, V'(\tau,u)\big)\big\rangle = \sum_{i=1}^{N} \int\limits_{\Sigma} f_i \left(C(u) f_i\right) dx',$$

where

$$f_i = \sqrt{\lambda_i} \sum_{j=1}^{N} d_{ij} x_j, \quad i = 1, \ldots, N, \tag{2.5}$$

if $A = (a_{ij})$ is transformed to the principal axis $DAD^* = \operatorname{diag}(\lambda_1, \ldots, \lambda_N)$ by unitary matrix $D = (d_{ij})$. Observe that $\lambda_1, \ldots, \lambda_N \geqslant 0$ since A is positive semi-definite. Thus, using the abbreviation

$$Q(u, f) = \int\limits_{\Omega} |\nabla \chi|^2 \, dx,$$

where $\chi = \chi(u, f)$ denotes the solution of the mixed BVP (2.3) with boundary values f, the effective potential (1.20) reads

$$J(u) = \sum_{i=1}^{N} Q(u, f_i) + U(u). \tag{2.6}$$

Since the special form of the boundary values in (2.5) is insignificant, in the following, we assume the data f_i to be arbitrary smooth functions, bounded on $\mathbb{R}^N$ together with their derivatives.

From now we concentrate on the stationary states relative to the effective potential (2.6). In particular, we seek to minimize J on a set of admissible shapes Ω with a volume constraint $|\Omega| = c_0$. Thus, we are faced with the optimal shape design problem

$$\text{find } u \in K \text{ with } P(u) \leqslant P(w) \text{ for all } w \in K, \tag{P}$$

where K is a subset of

$$W = \left\{ w \in C_+^{0,1}(\bar{B}) \mid \textstyle\int_B w \, dx = c_0 \right\}.$$

$C_+^{0,1}(\bar{B})$ denotes the cone of positive Lipschitz continuous functions. We set $\tilde{\chi} = \tilde{\chi}(u, f) = \chi - f$ which has a trace zero on Σ. Hence

$$\tilde{\chi} \in \widetilde{H}^1(\Omega) := \left\{ \varphi \in H^1(\Omega) \mid \varphi|_\Sigma = 0 \right\}$$

and

$$\int\limits_{\Omega} \nabla \tilde{\chi} \nabla \varphi \, dx = -\int\limits_{\Omega} \nabla f \nabla \varphi \, dx \ \text{ for all } \ \varphi \in \widetilde{H}^1(\Omega) \tag{2.7}$$

in view of (2.3). The particular choice $\varphi = \tilde{\chi}$ in (2.7) leads to the estimate

$$\|\tilde{\chi}(u, f)\|_{H^1(\Omega)}, \, \|\chi(u, f)\|_{H^1(\Omega)} \leqslant C(f, B) \left(\|u\|^2_{L^\infty(B)} + 1 \right) \tag{2.8}$$

if Poincare's inequality is remembered. We point finally to

$$Q(u, f) = \min_{\varphi \in \widetilde{H}^1(\Omega)} \int\limits_{\Omega} |\nabla(\varphi + f)|^2 \, dx = \int\limits_{\Omega} \left(|\nabla f|^2 - \nabla f \nabla \tilde{\chi} \right) dx$$

in consequence of the corresponding variational equations.

The effective potential J is continuous in the following sense: for any sequence $\{u_n\}_{n\geqslant 1}$, $u_n \in C^{0,1}_+(\bar{B})$ convergence $u_n \to u \in C^{0,1}_+$ in $C^0(\bar{B})$ implies $J(u_n) \to J(u)$. (For similar features of related shape functionals see [10, 19]). In fact, it suffices to verify continuity of the Dirichlet integral $Q(\cdot, f)$ with smooth f since the gravity part U of J is obviously even Lipschitz-continuous on $C^{0,1}(\bar{B})$. Extend the functions $\tilde{\chi}_n = \tilde{\chi}(u, f)$ across the upper boundaries $\Sigma_n = \Sigma_{u_n}$ by setting $\tilde{\chi}_n = 0$ outside their original domain $\Omega_n = \Omega_{u_n}$. In view of $\tilde{\chi}_n|_{\Sigma_n} = 0$ we may consider the extensions to belong to the Sobolev space $H^1(Z)$ where Z is a cylinder with a base B and a suitable chosen height h. Due to (2.8) the sequence is bounded in $H^1(Z)$. Then along every weakly convergent subsequence (again denoted by $\tilde{\chi}_n$): $\tilde{\chi}_n \rightharpoonup \psi$ in $H^1(Z)$

$$\lim_{n\to\infty} Q(u_n, f) = \lim_{n\to\infty} \Bigg(\int\limits_{\Omega_n} |\nabla f|^2 \, dx - \int\limits_{Z} \nabla f \nabla \tilde{\chi}_n \, dx \Bigg) = \int\limits_{\Omega} |\nabla f|^2 \, dx - \int\limits_{Z} \nabla f \nabla \psi \, dx.$$

It remains to show that $\psi|_\Omega$ belongs to $\widetilde{H}^1(\Omega)$ and satisfies (2.7), hence $\psi|_\Omega = \tilde{\chi}(u, f)$. But this becomes clear on passing to the limit in

$$\int\limits_{\Omega} \nabla \tilde{\chi}_n \nabla \varphi \, dx = -\int\limits_{\Omega} \nabla f \nabla \varphi \, dx \quad \text{for all } \varphi \in \widetilde{C}^\infty(\Omega) \text{ and } n \geqslant n_\varphi$$

and by observing that $\tilde{\chi}|_{Z\setminus\Omega} = 0$. Here $\widetilde{C}^\infty(\Omega)$ denotes the set of all functions $\varphi \in C^\infty(\Omega) \cap \widetilde{H}^1(\Omega)$ such that $\operatorname{supp}\varphi \subseteq \bar{\Omega}_{u-\varepsilon}$ for some $\varepsilon = \varepsilon_\varphi > 0$.

As an immediate consequence we notice

Proposition 2.1. *If $K \subset W$ is non-empty and compact in C^0, then there is at least one solution of the problem* (P). □

Remark 2.1. In general, in Proposition 2.1, we cannot exclude the minimizer to lie on the boundary of the admissibility set. Without further restrictive assumptions it seems difficult to get conditions that guarantee the minimizer to belong to the interior and to satisfy the free boundary condition (2.18). In Section 3, this question is settled locally, at least relative to periodic boundary conditions.

Next we study the smoothness of J and compute its first and second derivatives in a rigorous way. This is achieved by transforming the variable domains and the related Dirichlet intgrals onto a fixed reference domain. If $u, w \in C^{0,1}_+(\bar{B})$, $v = w - u$ and $\tilde{v} : \Omega \to \mathbb{R}$ is given by

$$\tilde{v}(x) = x_N v(x')/u(x'), \tag{2.9}$$

then the mapping

$$\Phi = \Phi(u, w) : x \mapsto x + \tilde{v}(x) e_N, \quad e_N = (0, \dots, 0, 1) \tag{2.10}$$

defines a bijective, i.e., differentiable mapping from Ω_u onto Ω_w. If we set

$$(g_{ij}) = (\partial_i \Phi \cdot \partial_j \Phi), \quad g = \det(g_{ij}), \quad (g^{ij}) = (g_{ij})^{-1}$$

or explicitly,

$$\sqrt{g}g^{ij} = (1 + \partial_N \tilde{v})\,\delta_{ij} - \partial_i \tilde{v}\,\delta_{Nj} - \partial_j \tilde{v}\,\delta_{Ni} + (1 + \partial_N \tilde{v})^{-1} |\nabla \tilde{v}|^2\,\delta_{Ni}\delta_{Nj}, \tag{2.11}$$

we get

$$Q(w, f) = \int\limits_\Omega \sqrt{g}g^{ij} \partial_i \psi \partial_j \psi\, dx, \tag{2.12}$$

where $\psi = \chi(w, f) \circ \Phi(u, w)$ is the pull-back of $\chi(w, f)$.

Proposition 2.2. *Let $f \in C^\infty(\mathbb{R}^N)$. Then the map $C^{0,1}_+(\bar{B}) \ni u \mapsto Q(u, f)$ is smooth. In particular, its first Fréchet derivative with respect to u reads*

$$Q'(u, f)v = \int\limits_\Omega \Big(|\nabla\chi|^2 \partial_N \tilde{v} - 2\partial_N \chi \nabla\chi \nabla\tilde{v} + 2\nabla\chi\nabla(\partial_N f \tilde{v}) \Big)\, dx, \tag{2.13}$$

where $\tilde{v}$ is defined by (2.9).

Proof. Fix $u \in C^{0,1}_+(\bar{B})$ and a sufficiently small neighbourhood M of u in $C^{0,1}(\bar{B})$. Then for $w \in M$ the pull-back $\tilde{\psi} = \tilde{\chi}(w, f) \circ \Phi(u, w)$ is the unique solution in $\widetilde{H}^1(\Omega)$ of

$$\int\limits_\Omega \sqrt{g}g^{ij} \partial_i \tilde{\psi} \partial_j \varphi\, dx = -\int\limits_\Omega \sqrt{g}g^{ij} \partial_i h \partial_j \varphi\, dx \;\text{ for all }\; \varphi \in \widetilde{H}^1(\Omega). \tag{2.14}$$

with $h = f \circ \Phi(u, w)$. The ellipticity and the smooth dependence

$$[w \mapsto \sqrt{g}g^{ij}],\; [w \mapsto \partial_i h] \in C^\infty\big(M, L^\infty(\Omega)\big),$$

of the coefficients and the right-hand side on $w \in M$, via the implicit function theorem, imply the solution $\tilde{\psi}$ of (2.14), in dependence on w, to belong to

$$[w \mapsto \tilde{\psi}] \in C^\infty\big(M, \widetilde{H}^1(\Omega)\big).$$

Thus, $Q(u, f)$ varies smoothly with $u \in C^{0,1}_+(\bar{B})$. Now, by differentiating (2.12) we get

$$Q'(w, f) = \int\limits_\Omega (\sqrt{g}g^{ij})' \partial_i \psi \partial_j \psi\, dx + 2\int\limits_\Omega \sqrt{g}g^{ij} \partial_i \psi \partial_j \psi'\, dx, \tag{2.15}$$

where a prime indicates differentiation in w. Because of $\tilde{\psi}' = \psi' - h' \in \widetilde{H}^1(\Omega)$ we have further

$$\int\limits_\Omega \sqrt{g}g^{ij} \partial_i \psi \partial_j \psi'\, dx = \int\limits_\Omega \sqrt{g}g^{ij} \partial_i \psi \partial_j h'\, dx. \tag{2.16}$$

Hence, inserting the derivatives

$$h'\{v\} = \partial_N f \tilde{v}, \quad \big(\sqrt{g}g^{ij}\big)'\{v\} = \delta_{ij}\,\partial_N \tilde{v} - \delta_{Nj}\,\partial_i \tilde{v} - \delta_{Ni}\,\partial_j \tilde{v}, \tag{2.17}$$

at $w = u$ into (2.15), (2.16), we get (2.13) immediately. □

Remark 2.2. Formula (2.13), via (2.8), implies the Lipschitz continuity of J in $C^{0,1}_+(\bar{B})$.

In view of $\chi \in C^\infty(\Omega)$ the integrand in (2.13) can be written as

$$|\nabla\chi|^2\partial_N\tilde{v} - 2\partial_N\chi\nabla\chi\nabla\tilde{v} + 2\nabla\chi\nabla(\partial_N f\tilde{v}) = \partial_N\big(|\nabla\chi|^2\tilde{v}\big) - 2\nabla\big(\nabla\chi\partial_N\tilde{\chi}\tilde{v}\big).$$

Assuming additionally $\chi \in C^1(\bar{\Omega})$, after integrating by parts, $Q'(u,f)v$ may be expressed as integral over Σ

$$Q'(u,f)v = \int_\Sigma \big(|\nabla f|^2 - |\nabla\tilde{\chi}|^2\big)\, v\, dx'.$$

This means that within the class of sufficiently regular solutions every critical point of J, under a volume constraint $|\Omega| = \text{const}$, satisfies the free boundary condition

$$\sum_{i=1}^N \big(|\nabla f_i|^2 - |\nabla\tilde{\chi}_i|^2\big) + b\cdot x = \text{const} \;\text{ on }\; \Sigma \tag{2.18}$$

with $\tilde{\chi}_i = \tilde{\chi}(u, f_i)$.

Proposition 2.3. *Maintaining the notation and assumptions of Proposition 2.2, the second derivative of Q reads*

$$Q''(u,f)\{v^2\} = 2\int_\Omega I\, dx, \tag{2.19}$$

where we have set

$$I = \nabla\chi\Big(\nabla\big(\tilde{v}^2\partial_N^2 f\big) + 2\big(\partial_N\tilde{v}\nabla\chi' - \partial_N\chi'\nabla\tilde{v}\big)\Big) + \big|\nabla\chi' - \partial_N\chi\nabla\tilde{v}\big|^2.$$

Here $\chi' = \psi'\{v\}$ denotes the derivative of $\psi = \chi(w,f)\circ\Phi(u,w)$ with respect to w at $w = u$.

Proof. Differentiating (2.12) twice in w at $w = u$ gives

$$Q''(u,f)\{v^2\} = \int_\Omega \Big((\sqrt{g}g^{ij})''\partial_i\chi\partial_j\chi + 4(\sqrt{g}g^{ij})'\partial_i\psi'\partial_j\chi + (\nabla\psi\nabla\psi)''\Big)\, dx.$$

Using $\tilde{\psi}'' = \psi'' - h'' \in \widetilde{H}^1(\Omega)$ and $h''\{v^2\} = \partial_N^2 f\tilde{v}^2$ at $w = u$, we obtain

$$\int_\Omega (\nabla\psi\nabla\psi)''\, dx = 2\int_\Omega |\nabla\psi'|^2\, dx + 2\int_\Omega \nabla\chi\nabla(\partial_N^2 f\tilde{v}^2)\, dx.$$

In view of (2.11), there holds

$$\big(\sqrt{g}g^{ij}\big)''\{v^2\} = 2\big|\nabla\tilde{v}\big|^2\delta_{iN}\delta_{jN},$$

hence

$$\int_\Omega \big(\sqrt{g}g^{ij}\big)''\partial_i\chi\partial_j\chi\, dx = 2\int_\Omega \big(\partial_N\chi\big)^2|\nabla v|^2\, dx.$$

Further, remembering (2.17), we have

$$\int_\Omega \big(\sqrt{g}g^{ij}\big)'\partial_i\chi\partial_j\psi'\, dx = \int_\Omega \Big(\nabla\chi\big(\nabla\psi'\partial_N\tilde{v} - \partial_N\psi'\nabla\tilde{v}\big) - \partial_N\chi\nabla\psi'\nabla\tilde{v}\Big)\, dx.$$

Adding the results shows the claim. □

Remark 2.3. Differentiating (2.14) and using (2.17), it is easily seen that

$$\int_\Omega \nabla\chi'\nabla\varphi\,dx = \int_\Omega \Big(\big(\partial_N\chi\nabla\tilde{v} - \nabla\chi\partial_N\tilde{v}\big)\nabla\varphi + \nabla\chi\nabla\tilde{v}\partial_N\varphi\Big)\,dx \tag{2.20}$$

for all $\varphi \in \widetilde{H}^1(\Omega)$. Together with the boundary condition $\chi' = \partial_N f\tilde{v}$ on Σ this determines χ' uniquely.

The integrand in (2.19) can be written

$$2\big|\nabla(\chi'-\tilde{v}\partial_N\chi)\big|^2 - 4\nabla\big(v\nabla\chi\partial_N\tilde{\chi}'\big) - 2\nabla\big(\nabla\partial_N\chi\partial_N\tilde{\chi}\tilde{v}^2\big) + 4\partial_N\big(v\nabla\chi\nabla\tilde{\chi}'\big) + 2\partial_N\big(\tilde{v}^2\nabla\chi\nabla\partial_N f\big).$$

Under the additional assumption $\partial_N\chi \in C^1(\bar{\Omega})$ this leads, via integration by parts, to

$$Q''(u,f)\{v^2\} = 2\int_\Omega \big|\nabla(\chi' - \tilde{v}\partial_N\chi)\big|^2\,dx + 2\int_\Sigma \big(\nabla\chi\nabla\partial_N f - \nabla\partial_N\chi\nabla\tilde{\chi}\big)\tilde{v}^2\,dx'$$

remembering $\tilde{\chi} = 0$, $\tilde{\chi}' = 0$ on Σ as well as $\tilde{v} = 0$ for $x_N = 0$. (For a rigorous proof $\tilde{\chi}'$ is to be approximated in $H^1(\Omega)$ by smooth functions vanishing near Σ). Moreover, as seen from (2.20)

$$\int_\Omega \nabla(\chi' - \tilde{v}\partial_N\chi)\nabla\varphi\,dx = \int_\Omega \nabla(\tilde{\chi}' - \tilde{v}\partial_N\tilde{\chi})\nabla\varphi\,dx = 0$$

for all $\varphi \in \widetilde{H}^1(\Omega)$. Thus, introducing the notation

$$|\psi|^2_{H^{1/2}(\Sigma)} := \min\left\{\int_\Omega |\nabla\varphi|^2\,dx \mid \varphi \in H^1(\Omega), \varphi|_\Sigma = \psi|_\Sigma\right\}$$

and remembering

$$|\psi|^2_{H^{1/2}(\Sigma)} = \int_\Sigma \psi\big(C(u)\psi\big)\,dx'$$

with the Dirichlet-Neumann operator $C(u)$ introduced earlier, we obtain

$$Q''(u,f)\{v^2\} = \int_\Sigma \Big(\tilde{v}\partial_N\tilde{\chi}\big(C(u)\tilde{v}\partial_N\tilde{\chi}\big) + \partial_N\big(|\nabla f|^2 - |\nabla\tilde{\chi})\tilde{v}^2\Big)\,dx'. \tag{2.21}$$

Corollary 2.4. *Let $u \in C^{0,1}_+(\bar{B})$ such that $\partial_N\tilde{\chi}_i \in C^1(\bar{\Omega})$, where $\tilde{\chi}_i = \tilde{\chi}(u,f_i)$, $i = 1,\dots,N$. Then the second variation $J''(u)$ turns out to be lower semi-bounded in $L^2(B)$, i.e., there holds*

$$J''(u)\{v^2\} \geqslant \alpha\|v\|^2_{L^2(B)}$$

for all $v \in C^{0,1}(\bar{B})$, where α is any real constant satisfying

$$\sum_{i=1}^N \partial_N\big(|\nabla f_i|^2 - |\nabla\tilde{\chi}_i|^2\big) + b_N \geqslant \alpha \quad \text{on} \quad \Sigma.$$

Moreover, if there exist $\xi_1,\dots,\xi_N \in \mathbb{R}$ such that $\sum_{i=1}^N \xi_i\partial_N\tilde{\chi}_i \geqslant c > 0$ on Σ, then there exists $\beta > 0$ with

$$J''(u)\{v^2\} \geqslant \alpha\|v\|^2_{L^2(B)} + \beta|\tilde{v}|^2_{H^{1/2}(\Sigma)} \tag{2.22}$$

for all $v \in C^{0,1}(\bar{B})$ and $\int_B v\,dx = 0$.

Proof. It remains to show (2.22). Let $\rho \in C^1(\bar{\Sigma})$ be any positive function. Then, if Friedrich's inequality is remembered, there holds

$$|\tilde{v}|^2_{H^{1/2}(\Sigma)} \leqslant C|\rho\tilde{v}|^2_{H^{1/2}(\Sigma)}$$

for all $v \in C^{0,1}(\bar{B})$ with $\int_B v\,dx = 0$. Thus, setting

$$\rho = \sum_{i=1}^N \xi_i \partial_N \tilde{\chi}_i|_\Sigma \in C^1(\bar{\Sigma}), \quad \varphi = \sum_{i=1}^N \xi_i \tilde{\chi}_i' \in \widetilde{H}^1(\Omega),$$

we obtain

$$|\rho\tilde{v}|^2_{H^{1/2}(\Sigma)} \leqslant \int_\Omega \big|\nabla(\varphi - \rho\tilde{v})\big|^2\,dx \leqslant C\sum_{i=1}^N \int_\Omega \big|\nabla(\chi_i' - \partial_N\chi_i\tilde{v})\big|^2\,dx$$

from which the result follows. □

3. Local stability result

In this section, assuming B to be a $(N-1)$-dimensional torus $\mathbb{T}$, we are interested in local minimizers of J under periodic boundary conditions. As usual $\mathbb{T}$ will be identified with the unit cube in $\mathbb{R}^{N-1}$. Necessarily, the given data are to be assumed periodic too. Clearly, for $f_1 = \ldots = f_N \equiv 0$ and $b_1 = \ldots = b_{N-1} = 0$, every planar surface $u = \text{const} > 0$ defines a critical point of J relative to some volume constraint. The following theorem shows the existence of smooth minimizers - represented by nearly planar surfaces -, for small data $\|f_i\|$ or, equivalently, for large values of b_N.

Theorem 3.1. *Let $f_1, \ldots, f_N \in C^\infty(\mathbb{T}\times\mathbb{R})$ and $b_1 \ldots, b_{N-1} = 0$. Then for b_N sufficiently large there exists a strong local minimizer $u \in C^\infty(\mathbb{T})$ of J with respect to a volume constraint $|\Omega| = const$. In particular, the free boundary condition* (2.18) *on Σ is met.*

A more sophisticated perturbation result in this context reads as follows: if u is a smooth critical point of J which belongs to smooth data $f_1, \ldots, f_N$ such that $J''(u)$ is non-degenerated and

$$\sum_{i=1}^N \partial_N\big(|\nabla f_i|^2\big) + b_N > 0 \quad \text{on} \quad \Sigma,$$

then, for any small perturbation of the data, there exist critical points in the neighbourhood of u. The proof of this latter variant runs nearly along the same lines as that of Theorem 3.1, but needs more technical effort. Furthermore, to avoid troublesome regularity checks, Theorem 3.1 is formulated in the C^∞-setting. In particular, the estimates shown in Lemmas 3.1 and 3.2 below turn out to be sufficient for our use, but can be strongly improved.

We use the notations of Section 2. Throughout this section let $u_0 \equiv 1$, $\Omega := \Omega_{u_0}$ and N_s be the set

$$N_s = \big\{u \in H^s(\mathbb{T}) \,\big|\, \|u - u_0\|_s \leqslant \delta_s\big\}$$

with $\delta_s > 0$ sufficiently small. Note that $N_s \subset C_+^{0,1}(\mathbb{T})$ for $s > (N+1)/2$ by Sobolev's embedding.

Lemma 3.1. *Let $k \geqslant 1$ be an integer, $s > (N+1)/2$ and $f \in C^\infty(\mathbb{T}\times\mathbb{R})$. Then there exists a constant $C > 0$ depending on k, s, δ_s and f such that for all $u \in N_s$ and $u_1, \ldots, u_k \in C^\infty(\mathbb{T})$ there holds*

$$\left|Q^{(k)}(u,f)\{u_1,\ldots,u_k\}\right| \leqslant C\|u_1\|_{1/2}\|u_2\|_{1/2}\|u_3\|_s\cdots\|u_k\|_s. \tag{3.1}$$

Proof. Set $\sigma = s-1/2$. Because of $\sigma > N/2$ the spaces $H^\sigma(\Omega)$ turn into Banach algebras. The composition of the C^∞-functions with the H^σ-functions leads to H^σ-functions again, e.g., $F \in C^\infty(\mathbb{T}\times\mathbb{R})$ and $w \in H^\sigma(\Omega)$ imply $F(\cdot, w(\cdot)) \in H^\sigma(\Omega)$ and there holds

$$\|F(\cdot, w(\cdot))\|_\sigma^\Omega \leqslant C \tag{3.2}$$

for all w from the bounded subsets of $H^\sigma(\Omega)$ with constants depending on σ, F, and the upper bounds of $\|w\|_\sigma^\Omega$. In particular, we have

$$\|1/w\|_\sigma^\Omega \leqslant C(\alpha, \|w\|_\sigma) \tag{3.3}$$

for all $w \in H^\sigma(M)$ with $w \geqslant \alpha > 0$ on Ω. Concerning the pointwise multiplication, we quote

$$\|v\cdot w\|_t^\Omega \leqslant C\|v\|_t^\Omega\|w\|_\sigma^\Omega \tag{3.4}$$

for $0 \leqslant t \leqslant \sigma$, $v \in H^t(\Omega)$ and $w \in H^\sigma(\Omega)$.

For $u = u_0 + v \in N_s$ let Φ be the bijective mapping from Ω onto Ω_u as defined in (2.10), but now with the more sophisticated definition

$$\tilde{v}(x) = \tilde{v}(x', x_N) := x_N \mathscr{E} v(x', x_N - 1)$$

where $\mathscr{E}v$ with $\mathscr{E}v|_{\mathbb{T}} = v$ is an extension of v into $\mathbb{T}\times\mathbb{R}$. According to the trace mapping theorem, we can choose $\mathscr{E} \in \mathscr{L}\big(H^t(\mathbb{T}), H^t(\mathbb{T}\times\mathbb{R})\big)$ for all $t > 0$, hence

$$\|\tilde{v}\|_{t+1/2}^\Omega \leqslant C\|v\|_t. \tag{3.5}$$

For sufficiently small $\delta_s > 0$, we have $\partial_N\tilde{v} > -1$ in Ω, hence T yields a bijective mapping from Ω onto Ω_u for all $u \in N_s$. In view of (2.11) we have now

$$[u \mapsto \sqrt{g}g^{ij}], [u \mapsto \nabla(f\circ\Phi)] \in C^\infty\big(N_s, H^\sigma(\Omega)\big).$$

More precisely, as $\delta^k\sqrt{g}g^{ij}$ is a polynomial in the first derivatives of $\tilde{u}, \ldots, \tilde{u}_k$ and $1/(1+\partial_N\tilde{u})$ by (3.3), (3.4) we are led to

$$\left\|\left(\sqrt{g}g^{ij}\right)^{(k)}\{u_1,\ldots,u_k\}\right\|_t^\Omega \leqslant C\|\tilde{u}_1\|_{t+1}^\Omega\|\tilde{u}_2\|_{s+1/2}^\Omega\cdots\|\tilde{u}_k\|_{s+1/2}^\Omega$$

for $0 \leqslant t \leqslant \sigma$. Remembering (3.5), we obtain

$$\left\|\left(\sqrt{g}g^{ij}\right)^{(k)}\{u_1,\ldots,u_k\}\right\|_t^\Omega \leqslant C\|u_1\|_{t+1/2}\|u_2\|_s\cdots\|u_k\|_s. \tag{3.6}$$

By the same reasoning we get additionally, if $k \geqslant 2$,

$$\left\|\left(\sqrt{g}g^{ij}\right)^{(k)}\{u_1,\ldots,u_k\}\right\|_{L^1(\Omega)} \leqslant C\|u_1\|_{1/2}\|u_2\|_{1/2}\|u_3\|_s\cdots\|u_k\|_s. \tag{3.7}$$

Considering

$$(f\circ\Phi)^{(k)}\{u_1,\ldots,u_k\} = \big((\partial_N^k f)\circ\Phi\big)\cdot\tilde{u}_1\cdots\tilde{u}_k$$

and (cf. (3.2))

$$\|(\partial_N^k f)\circ\Phi\|_{\sigma+1}^{\Omega}\leqslant C,$$

we obtain similarly

$$\big\|(f\circ\Phi)^{(k)}\{u_1,\dots,u_k\}\big\|_{t+1}^{\Omega}\leqslant C\|u_1\|_{t+1/2}\|u_2\|_s\cdots\|u_k\|_s \tag{3.8}$$

for all $0\leqslant t\leqslant\sigma$, as well as

$$\big\|\nabla(f\circ\Phi)^{(k)}\{u_1,\dots,u_k\}\big\|_{L^1(\Omega)}\leqslant C\|u_1\|_{1/2}\|u_2\|_{1/2}\|u_3\|_s\cdots\|u_k\|_s. \tag{3.9}$$

Now, $\tilde\psi=\tilde\psi(u,f):=\tilde\chi(u,f)\circ\Phi$ being the solution of (2.14), the elliptic regularity theory implies via the perturbation arguments

$$\|\tilde\psi(u,f)\|_{\sigma+1}^{\Omega}\leqslant C \tag{3.10}$$

for all $u\in N_s$. As for the derivatives $\tilde\psi^{(k)}$, differentiation of (2.14) implies in view of (3.6), (3.8) by the induction

$$\|\tilde\psi^{(k)}(u,f)\{u_1,\dots,u_k\}\|_{t+1}^{\Omega}\leqslant C\|u_1\|_{t+1/2}\|u_2\|_s\cdots\|u_k\|_s \tag{3.11}$$

for $0\leqslant t\leqslant\sigma$. Finally, differentiating the expression

$$Q'(u,f)v=\int\limits_{\Omega}\big((\sqrt{g}g^{ij})'v\big)\partial_i\psi\partial_j\psi\,dx+2\int\limits_{\Omega}\sqrt{g}g^{ij}\partial_i\psi\partial_j\big(f\circ T)'v\big)\,dx$$

$k-1$ times in u and considering estimates (3.6), (3.8), (3.11) with $t=0$ or $t=\sigma$ as well as (3.7), (3.9) implies the assertion. □

Translation invariant Q means that for any translation $T'_\tau : x'\mapsto x'+\tau$ with $\tau'=(\tau_1,\dots,\tau_{N-1})\in\mathbb{R}^{N-1}$ there holds

$$\chi\big(u\circ T_{\tau'},f\circ T_{\tau'}\big)=\chi(u,f)\circ T_{\tau'}$$

and consequently,

$$Q\big(u\circ T_{\tau'},f\circ T_{\tau'}\big)=Q(u,f).$$

Differentiating with respect to τ_i and remembering the quadratic character of Q in f implies

$$Q'(u,f)\partial_i u+2Q(u,f,\partial_i f)=0$$

for the corresponding quadratic form $Q(u,\cdot,\cdot)$, provided u, f are smooth. Repeated differentiation with respect to u leads to

$$\begin{aligned}Q^{(k)}(u,f)\{\partial u_1,u_2,\dots,u_k\}=&-\sum_{i=2}^{k}Q^{(k)}(u,f)\{u_1,\dots,\partial u_i,\dots,u_k\}\\&-Q^{(k+1)}(u,f)\{\partial u,u_1,\dots,u_k\}-2Q^{(k)}(u,f,\partial f)\{u_1,\dots,u_k\}\end{aligned} \tag{3.12}$$

for any partial derivative $\partial=\partial_i$, $i=1,\dots,N-1$. The latter formula copies integration by parts at an abtract level. This implies

$$\begin{aligned}Q^{(k)}(u,f)\{\partial u_1,u_1,u_3\dots,u_k\}=&-\frac12\sum_{i=3}^{k}Q^{(k)}(u,f)\{u_1,\dots,\partial u_i,\dots,u_k\}\\&-\frac12 Q^{(k+1)}(u,f)\{\partial u,u_1,\dots,u_k\}-Q^{(k)}(u,f,\partial f)\{u_1,\dots,u_k\}\end{aligned} \tag{3.13}$$

in the special case $u_1=u_2$, $k\geqslant 2$.

Lemma 3.2. *Let $f \in C^\infty(\mathbb{T} \times \mathbb{R})$ and $s \geqslant s_0 := N + 4$ be an integer. Then there exist constants C (independent of s) and C_s such that for all $u \in N_{s_0} \cap C^\infty(\mathbb{T})$ there holds*

$$Q'(u, f)\{\Delta^s u\} \geqslant -C\|u\|_s^2 - C_s$$

with the Laplacian $\Delta = -\sum_{i=1}^{N-1} \partial_i^2$.

Proof. From Sobolev's embedding $H^{s_0+1/2}(\Omega) \hookrightarrow C^2(\bar{\Omega})$ and (3.10) we obtain a uniform boundedness of $\chi(u, f)$ in $C^2(\bar{\Omega}_u)$ and, remembering (2.21),

$$Q''(u, f)\{v, v\} \geqslant -C\|v\|_0^2 \tag{3.14}$$

for all $u \in N_{s_0}$ and $v \in C^{0,1}(\mathbb{T})$. Applying the differentiation rule (3.12) to

$$Q'(u, f)\{\Delta^s u\} = (-1)^s \sum_{|\alpha|=s} Q'(u, f)\{\partial^\alpha \partial^\alpha u\}$$

we get

$$\begin{aligned} Q'(u, f)\{\Delta^s u\} &= \sum_{|\alpha|=s} Q''(u, f)\{\partial^\alpha u, \partial^\alpha u\} \\ &+ \sum_{|\alpha|=s} \sum_{k,\beta} a_{k,\beta} Q^{(k-1)}(u, \partial^{\beta_1} f, \partial^{\beta_2} f)\{\partial^{\beta_3} u, \ldots, \partial^{\beta_k} u, \partial^\alpha u\} \end{aligned} \tag{3.15}$$

with certain integers $a_{k,\beta}$, where the second sum extends over all integers $k \geqslant 2$ and systems of multiindices $\beta_1, \ldots, \beta_k$ with

$$|\beta_1| + \beta_2| + \ldots + |\beta_k| = s, \quad 1 \leqslant |\beta_3| \leqslant \ldots \leqslant |\beta_k| \leqslant s.$$

In view of (3.14) this implies

$$\sum_{|\alpha|=s} Q''(u, f)\{\partial^\alpha u, \partial^\alpha u\} \geqslant -C\|u\|_s^2 \tag{3.16}$$

with a constant C independent of s.

The second sum in (3.15) can be expressed as

$$\sum_{|\alpha|=s-1} \sum_{k,\beta} c_{k,\beta} Q^{(k-1)}(u, \partial^{\beta_1} f, \partial^{\beta_2} f)\{\partial^{\beta_3} u, \ldots, \partial^{\beta_k} u, \partial^\alpha u\} \tag{3.17}$$

where the sum runs over all integer $k \geqslant 2$ and systems of multiindices $\beta_1, \ldots, \beta_k$ with

$$|\beta_1| + \beta_2| + \ldots + |\beta_k| = s + 1, \quad 1 \leqslant |\beta_3| \leqslant \ldots \leqslant |\beta_k| \leqslant s - 1.$$

This can be achieved by shifting a single derivative ∂_l in $\partial^\alpha u$ to the remaining arguments. If $k = 2$ or $|\beta_k| \leqslant s - 2$, apply (3.12) to get the claim. Otherwise, use (3.13) to alter the position of ∂_l.

Setting $s = \sigma = 1 + N/2$ in (3.1) implies

$$|S| \leqslant C_s \|\partial^{\beta_3} u\|_\sigma \cdots \|\partial^{\beta_{k-1}} u\|_\sigma \|\partial^{\beta_k} u\|_{1/2} \|\partial^\alpha u\|_{1/2}$$

for a typical summand S of (3.17), where C_s, apart from s, depends on k and f. If $k = 2$ and $k = 3$, then

$$|S| \leqslant C_s \|u\|_{s-1/2} \quad \text{and} \quad |S| \leqslant C_s \|u\|_{s-1/2}^2$$

respectively. As to the remaining case $k \geqslant 4$: if $|\beta_k| < \sigma + 2$ or $|\beta_{k-1}| < 2$, then $|\beta_i| + \sigma \leqslant 2\sigma + 2 = s_0$, $i = 3, \dots, k-1$, which implies

$$|S| \leqslant C_s \|u\|_{s_0}^{k-3} \|u\|_{s-1/2}^2.$$

Alternatively, if $|\beta_k| \geqslant \sigma + 2$, $|\beta_{k-1}| \geqslant 2$, choose $l \geqslant 3$ to be the smallest index i with $|\beta_i| \geqslant 2$, then

$$|S| \leqslant C_s \|u\|_{\sigma+1}^{l-3} \|u\|_{d_l+\sigma+2} \dots \|u\|_{d_k+\sigma+2} \|u\|_{s-1/2},$$

where $d_k = |\beta_k| - \sigma - 3/2 > 0$ and $d_i = |\beta_i| - 2 \geqslant 0$, $i = l \dots, k-1$. Because of

$$d := \sum_{i=l}^{k} d_i \leqslant \sum_{i=1}^{k} |\beta_i| - \sigma - 7/2 \leqslant s - \sigma - 5/2$$

we finally get

$$\|u\|_{d_l+\sigma+2} \dots \|u\|_{d_k+\sigma+2} \leqslant C_s \|u\|_{d+\sigma+2} \|u\|_{\sigma+2}^{k-l} \leqslant C_s \|u\|_{s-1/2} \|u\|_{s_0}^{k-l}$$

by norm convexity estimates. This shows an estimate of the type

$$|S| \leqslant \varepsilon \|u\|_s^2 + C(\varepsilon, s, \|u\|_{s_0}), \quad \varepsilon > 0$$

in every case. In view of (3.16) this proves the assertion. □

The proof of Theorem 3.1 is based on the following existence principle (cf. [13; Thm. I]):

Lemma 3.3. *Let V be a separable normed real vector space continuously and densely embedded into a reflexive real Banach space X. Further, let K be a bounded, closed and convex subset of X containing 0 as an interior point and F be a weakly sequentially continuous map of K into V' such that*

$$\langle F(v), v \rangle \geqslant 0 \quad \textit{for all} \quad v \in V \cap \partial K,$$

where ∂K denotes the boundary of K. Then there exists $u \in K$ with $F(u) = 0$, i.e., $\langle F(u), v \rangle = 0$ for all $v \in V$. □

Proof of Theorem 3.1. Let $s \geqslant s_0 := N + 4$ be an integer. In order to apply Lemma 3.3, we introduce the Banach space

$$X = \big\{ u \in H^s(\mathbb{T}) \mid \textstyle\int_{\mathbb{T}} u \, dx = 0 \big\}, \quad \|u\|_X^2 = \varepsilon_s^2 |u|_s^2 + |u|_{s_0}^2$$

with suitable small $\varepsilon_s > 0$ to be chosen later, and the (separable) normed space

$$V = C^\infty(\mathbb{T}) \cap X, \quad \| \cdot \|_V = \| \cdot \|_{2s+N}.$$

Here $| \cdot |_s$ abbreviates $|u|_s^2 = \sum_{|\alpha|=s} \|\partial^\alpha u\|_0^2$. Note that on X the norm $\| \cdot \|_X$ is equivalent to any other Sobolev norm $\| \cdot \|_s$. Define $K \subset X$ according to

$$K = \big\{ v \in X \mid \|v\|_X \leqslant \delta \big\}.$$

Because of $|u|_{s_0} \leqslant \|u\|_X$ we can choose a suitable $\delta > 0$ independent of s such that $u_0 + u \in N_{s_0}$ for all $u \in K$. Finally, $F : K \to V'$ is defined by

$$\langle F(u), v\rangle = J'(u_0 + u, f)\big\{\Delta^{s_0} v + \varepsilon_s^2 \Delta^s v\big\}.$$

Note that

$$\|\Delta^{s_0} v + \varepsilon_s^2 \Delta^s v\|_{C^{0,1}} \leqslant C_s \|v\|_V$$

for all $v \in V$ by Sobolev's embedding, hence in fact $F(u) \in V'$.

Noting that the mapping $\Delta^{s_0} + \varepsilon_s^2 \Delta^s : V \to V$ to be bijective, the existence of $u \in K$ with $F(u) = 0$ implies

$$J'(u_0 + u)v = 0 \quad \text{for all}\, v \in V,$$

which shows $u_0 + u$ to be critical relative to the volume constraint.

Show that F is weakly sequentially continuous. Let $\{u_n\}$, $u_n \in K$ be weakly convergent: $u_n \rightharpoonup u \in K$ in X. By the compact embedding $C^{0,1}(\mathbb{T}) \subset H^{s_0}(\mathbb{T})$ this implies the norm convergence $u_n \to u$ in $C^{0,1}(\mathbb{T})$. Thus, the smoothness of J on $C_+^{0,1}(\mathbb{T})$ yields

$$\lim_{n\to\infty} \langle F(u_n), v\rangle = \langle F(u), v\rangle \quad \text{for all}\, v \in V.$$

Noting that

$$\langle F(u), u\rangle = b_N\big(|u|_{s_0}^2 + \varepsilon_s^2 |u|_s^2\big) + \sum_{i=1}^N Q'(u_0 + u, f_i)\big\{\Delta^{s_0} u + \varepsilon_s^2 \Delta^s u\big\},$$

we obtain from Lemma 3.2 for $u \in K \cap V$

$$\langle F(u), u\rangle \geqslant (b_N - C_1)\|u\|_X^2 - C_2 - \varepsilon_s^2 C_s,$$

where the constants C_1, C_2 are independent of s. Hence choosing $\varepsilon_s = (C_2/C_s)^{1/2}$ and assuming $b_N \geqslant C_1 + 2C_2/\delta^2$, we get

$$\langle F(u), u\rangle \geqslant 0 \quad \text{for all}\, u \in V,\ \|u\|_X = \delta.$$

Now, the existence of $u \in K$ with $F(u) = 0$ is implied by Lemma 3.3.

Smoothness of the solution follows from the uniqueness, since the independence of $s \geqslant s_0$ implies $u \in C^\infty(\mathbb{T})$. In fact, assuming the existence of $u_1, u_2 \in K$ with $F(u_1) = F(u_2) = 0$ leads to

$$0 = J'(u_0 + u_1)w - J'(u_0 + u_2)w, \quad w = u_1 - u_2$$

and, in view of (3.14), to

$$b_N \|w\|_0^2 = -\sum_{i=1}^N \int_0^1 Q''(u_0 + u_2 + tw, f_i) w^2\, dt \leqslant C\|w\|_0^2,$$

where C is independent of s. If $b_N > C$, this implies $w = 0$. □

4. Finite element approximation

This section centers on finite element discretization of the functional J in dimensions $N = 2, 3$. We use piecewise linear elements to approximate the free boundary Σ. We refer first and foremost to $3D$; the differences from the two-dimensional case are only indicated, if not obvious. In the following, we assume $B \subset \mathbb{R}^2$ to be either a polygonal domain or, as in the periodic setting of Section 3, a two-dimensional torus $\mathbb{T}$. Let $\{\mathscr{T}_h^B\}$ denote a non-degenerate (or regular) family of triangulations of B by (closed) triangles in the usual sense (cf. [5; Definition 4.4.13]). This means that if h measures the maximal diameter of a triangle, then there exist constants $C_1, C_2 > 0$ independent of h such that for all triangles $T \in \mathscr{T}_h^B$

$$\operatorname{diam} T \leqslant C_1 h, \quad \operatorname{diam} B_T \geqslant C_2 \operatorname{diam} T,$$

where B_T denotes the largest disk contained in T. The triangulations are called quasi-uniform if the latter estimate can be replaced by $\operatorname{diam} B_T \geqslant C_2 h$. Let V_h^B be the space of piecewise linear elements belonging to $\mathscr{T}_h^B$, i.e.,

$$V_h^B = \big\{ v \in C^{0,1}(\bar{B}) \;\big|\; v|_T \in \mathscr{P}_1(T) \text{ for all } T \in \mathscr{T}_h^B \big\},$$

where $\mathscr{P}_1(T)$ denotes the space of restrictions to T of polynomials in two variables of degree $\leqslant 1$. If $\pi_h^B : C^0(\bar{B}) \to V_h^B$ is the corresponding interpolation operator then the interpolation error estimates read

$$\|u - \pi_h^B u\|_{L^\infty(B)} + h \| |u - \pi_h^B u\|_{W^{1,\infty}(B)} \leqslant Ch^2 \|u\|_{W^{2,\infty}(B)}. \tag{4.1}$$

For later use, we recall the (trivial) inverse estimates

$$\|u\|_{W^{1,\infty}(B)} \leqslant Ch^{-1} \|u\|_{L^\infty(B)} \leqslant Ch^{-2} \|u\|_{L^2(B)} \text{ for } u \in V_h^B \tag{4.2}$$

for a quasi-uniform family of triangulations $\{\mathscr{T}_h^B\}$. For $N = 2$, in the latter estimate, h^{-2} is to be replaced by $h^{-3/2}$.

Further, let $\{\mathscr{T}_h\}$ be a non-degenerate family of triangulations of the reference domain $\Omega_0 = B \times (0,1) \subset \mathbb{R}^3$ by tetrahedrons compatible with $\{\mathscr{T}_h^B\}$ in the following sense. For every tetrahedron $T \in \mathscr{T}_h$ there exists a triangle $T' \in \mathscr{T}_h^B$ such that T and its vertices, via orthogonal projection onto $x_3 = 0$, are mapped onto T' and its vertices, respectively. Such a triangulation may be obtained, e.g., by a suitable subdivision of every prism $P_T = T \times (0,1) \subset \mathbb{R}^3$, $T \in \mathscr{T}_h^B$ into in a number of tetrahedrons with equidistant vertices on the three vertical edges of the prism. Correspondingly, let π_h be the interpolation operator into the space of piecewise linear elements belonging to $\mathscr{T}_h$. Then for every positive $u \in V_h$

$$\Phi_h(u) : x \mapsto x + \tilde{u}_h e_3, \quad \tilde{u}_h := \pi_h\big(x_3(u-1)\big)$$

defines the bijective mapping from Ω_0 onto Ω_u such that for all $T \in \mathscr{T}_h$ the restriction $\Phi_h(u)|_T$ is an affine-linear mapping from T onto a tetrahedron contained in $\bar{\Omega}_u$. Thus,

$$\mathscr{T}_h^u = \big\{ \Phi_h(u)T \;\big|\; T \in \mathscr{T}_h \big\}, \quad u \in V_h,$$

defines the family of triangulations of Ω_u by tetrahedrons. Correspondingly, let π_h^u denote the interpolation operator into the space of piecewise linear elements belonging to $\mathscr{T}_h^u$. Note that

$$\pi_h^u \varphi = \pi_h\big(\varphi \circ \Phi_h(u)\big) \circ \Phi_h(u)^{-1}$$

by construction. For positive $u, w \in V_h$, let Φ_h denote the mapping

$$\Phi_h(u,w) = \Phi_h(w) \circ \Phi_h(u)^{-1} : x \mapsto x + \tilde{v}_h e_N, \quad \tilde{v}_h = \pi_h^u \tilde{v}, \tag{4.3}$$

where $v = w - u$ and $\tilde{v}$ is to be taken from (2.9). Φ_h defines the bijective, i.e., differentiable map from Ω_u onto Ω_w which transforms $\mathscr{T}_h^u$ into $\mathscr{T}_h^w$. Finally, for $m \geqslant 1$, let

$$W_h^u = \bigl\{\varphi \in C^{0,1}(\bar{\Omega}_u) \bigm| \varphi|_T \in \mathscr{P}_m(T) \text{ for all } T \in \mathscr{T}_h^u\bigr\}$$

be the space of finite elements of the order m over $\mathscr{T}_h^u$. With $\Pi_h^u : C^0(\Omega_u) \to W_h^u$ denoting the corresponding interpolation operator there holds

$$\|\varphi - \Pi_h^u\varphi\|_{L^\infty(T)} + h\|\varphi - \Pi_h^u\varphi\|_{W^{1,\infty}(T)} \leqslant Ch^{m+1}\|\varphi\|_{W^{m+1,\infty}(T)} \tag{4.4}$$

for all $T \in \mathscr{T}_h^u$. The constant C depends on u but is uniformly bounded for all u varying in a set of the form $\{u \in V_h \mid u \geqslant C_1, \|u\|_{C^{0,1}} \leqslant C_2\}$ with some positive constants C_1, C_2. Note that the mapping $\Phi_h(u,w)$ according to (4.3) transforms W_h^u into W_h^w, i.e.,

$$W_h^u = \bigl\{\psi \circ \Phi_h(u,w) \mid \psi \in W_h^w\bigr\}. \tag{4.5}$$

We are now prepared to approximate J relative to the spaces V_h and $\widetilde{W}_h^u = W_h^u \cap \widetilde{H}^1(\Omega_u)$. For given smooth functions f_i and positive $u \in V_h$ we set

$$J_h(u) = \sum_{i=1}^{N} Q_h(u, f_i) + U(u), \quad Q_h(u,f) = \int_{\Omega_u} \bigl|\nabla(\tilde{\chi}_h + f)\bigr|^2\,dx, \tag{4.6}$$

where $\tilde{\chi}_h = \tilde{\chi}_h(u,f) \in \widetilde{W}_h^u$ is the solution of

$$\int_{\Omega_u} \nabla\tilde{\chi}_h \nabla\varphi\,dx = -\int_{\Omega_u} \nabla f \nabla\varphi\,dx \text{ for all } \varphi \in \widetilde{W}_h^u. \tag{4.7}$$

Obviously,

$$Q(u,f) \leqslant Q_h(u,f) \leqslant \int_{\Omega_u} \bigl|\nabla(\varphi + f)\bigr|^2\,dx \text{ for all } \varphi \in \widetilde{W}_h^u.$$

Since the nodes of the triangulations $\mathscr{T}_h^u$, for fixed h, depend smoothly on $u \in V_h$, the stiffness matrix of (4.7) as well as its right side varies smoothly on u. Hence $J_h(u)$ varies smoothly in $u \in V_h$ as long as u remains positive. Moreover, J_h defines a consistent discretization of J in the following sense:

Lemma 4.1. *For any sequence $u_h \in V_h$, which is uniformly bounded in $C^{0,1}$, convergence $u_h \to u \in C_+^{0,1}(\bar{B})$ in C^0 implies $J_h(u_h) \to J(u)$.*

Proof. It suffices to verify the property for Q_h. For given $\varepsilon > 0$ we approximate $\tilde{\chi} = \tilde{\chi}(u,f)$ in $H^1(\Omega_u)$ by a smooth function φ vanishing in $Z \setminus \Omega_{u-\delta}$ with $\delta \in (0,\varepsilon)$ such that

$$\int_{\Omega_u} |\nabla(\varphi + f)|^2\,dx \leqslant Q(u) + \varepsilon.$$

Since $\Omega_{u-\delta} \subset \Omega_{u_h}$ and $\|u - u_h\|_{C^0} \leqslant \varepsilon$ for h sufficiently small, we obtain from (4.4) and the uniform boundedness of $\{u_h\}$ in $C^{0,1}$

$$\lim_{h\to 0} \|\nabla(\varphi_h - \varphi)\|_{L^\infty(\Omega_h)} = 0, \quad \varphi_h := \pi_h^{u_h}\varphi \in \widetilde{W}_h^{u_h},$$

and, additionally,

$$Q_h(u_h, f) \leqslant \int\limits_{\Omega_{u_h}} \left|\nabla(\varphi_h + f)\right|^2 dx \leqslant \int\limits_{\Omega_{u-\varepsilon}} \left|\nabla(\varphi_h + f)\right|^2 dx + C\varepsilon.$$

Hence

$$\lim_{h\to 0} \int\limits_{\Omega_{u-\delta}} \left|\nabla(\varphi_h + f)\right|^2 dx = \int\limits_{\Omega_{u-\delta}} \left|\nabla(\varphi + f)\right|^2 dx \leqslant \int\limits_{\Omega_u} \left|\nabla(\varphi + f)\right|^2 dx$$

and

$$\limsup_{h\to 0} Q_h(u_h, f) \leqslant Q(u, f) + C\varepsilon$$

for all $\varepsilon > 0$ with a constant independent of ε. On the other hand, remembering the continuity of Q as stated in Section 2, we have

$$Q(u, f) = \lim_{h\to 0} Q(u_h, f) \leqslant \liminf_{h\to 0} Q_h(u_h, f),$$

which finishes the proof of the consistency property. □

With the abbreviation $K_h = K \cap V_h$ we replace the minimum problem (P) by the sequence of discretized problems

$$\text{find } u_h \in K_h \text{ with } J_h(u_h) \leqslant J_h(w) \text{ for all } w \in K_h \tag{P_h}$$

in V_h.

Proposition 4.1. *Let $K \subset W$ as in Proposition 2.1 and $v \in K$ be a minimizer of* (P) *such that there exists $v_h \in K \cap V_h$, $0 < h < h_0$, with*

$$\sup\nolimits_{0<h<h_0} \|v_h\|_{C^{0,1}} < +\infty, \quad v_h \to v \text{ in } C^0(\bar{B}) \text{ as } h \to 0.$$

Then there are minimizers $u_h \in K_h$, $0 < h < h_0$ of (P_h). Additionally, we have $J_h(u_h) \to J(u)$ as well as $u_h \to u$ in C^0 for a suitable subsequence with $u \in K$ is minimizer of (P).

Proof. Being smooth on a compact non-empty set K_h, $0 < h < h_0$, the functional J_h has a minimizer $u_h \in K_h$. Compactness of K in C^0 implies convergence $u_h \to u \in K$ in C^0 for a suitable subsequence. In view of $J(u_h) \leqslant J_h(u_h) \leqslant J_h(v_h)$ and of $J_h(v_h) \to J(v)$ (cf. Lemma 4.1) it follows that $J(u) \leqslant \liminf J(u_h) \leqslant J(v)$, which shows u to be a minimizer of (P). □

Computation of the derivative $Q'_h(u, f)$ runs along the lines outlined in Section 2 by means of $Q'(u, f)$. Relate Ω_w via $\Phi_h(u, w)$ to the reference domain Ω_u and remember (4.5) in order to get, parallel with (2.13), the following proposition.

Proposition 4.2. *For positive $u \in V_h$ and $v \in V_h$, the first derivative of Q_h with respect to u reads*

$$Q'_h(u,f)v = \int\limits_\Omega \Big(|\nabla \chi_h|^2 \partial_N \tilde{v}_h - 2\partial_N \chi_h \nabla \chi_h \nabla \tilde{v}_h + 2\nabla \chi_h \nabla(\partial_N f \tilde{v}_h)\Big)\, dx, \tag{4.8}$$

where $\chi_h = \tilde{\chi}_h + f$, $\tilde{v}_h = \pi_h^u \tilde{v} : \Omega \to \mathbb{R}$ and $\tilde{v}$ is taken from (2.9). □

For $m = 1$ and linear f formula (4.8) simplifies. If V_T denotes the set of vertices of $T \in \mathscr{T}_h^u$, then

$$Q'_h(u,f)v = \frac{1}{N+1} \sum_{T \in \mathscr{T}_h^u} |T| \sum_{p \in V_T} \tilde{v}_h(p) \nabla \chi_h \big(\nabla \chi_h \partial_N \phi_p - 2\partial_N \tilde{\chi}_h \nabla \phi_p\big), \tag{4.9}$$

where $\phi_p \in W_h^u$ is chosen according to $\phi_p(q) = \delta_{pq}$ for $p, q \in V_T$ (see [17; Chapter 7], for similar calculations).

Remark 2.1 applies to the discrete problems (P_h) as well. The minimizer $u_h \in K_h$ cannot be excluded to belong to the boundary of K_h. Moreover, there is no information about the error $\|u - u_h\|$. The next theorem, which is the main result of this section, fills this gap in dimensions $N = 2, 3$. The estimate requires additional regularity of u which is guaranteed, e.g., by the results of Section 3, under periodic boundary conditions. In the following, we assume the triangulation $\mathscr{T}_h^B$ to be quasi-uniform.

Theorem 4.3. *Let $u \in W \cap C^3(\bar{B})$ be a local minimizer of* (P) *such that $\partial_N^k \tilde{\chi}_i \in C^1(\bar{\Omega})$ for $k = 0, \dots, 3$, where we have set $\tilde{\chi}_i = \tilde{\chi}(u, f_i)$, $i = 1, \dots, N$. If there is stability in the sense*

$$b_N > \sum_{i=1}^N \partial_N \big(|\nabla \tilde{\chi}_i|^2 - |\nabla f_i|^2\big) \quad on \quad \Sigma,$$

then, for $N = 2, 3$ and $m \geqslant 2$, there exist $h_0 > 0$ and a local minimizer $u_h \in W \cap V_h$, $0 < h < h_0$, of (P_h) with

$$\|u - u_h\|_{L^2} \leqslant C h^{3/2}.$$

For $N = 2$ and $m = 1$ the exponent is to be replaced by 1.

The proof of Theorem 4.3, which is given at the end of this section, is essentially contained in Propositions 4.4, 4.5. In both propositions we assume u to be a local minimizer of J with smoothness and stability as in Theorem 4.3.

Proposition 4.4. *For each $L > 0$, there exist $\delta > 0$ and $\alpha > 0$ such that*

$$\sum_{i=1}^N Q(w, \varphi_i, f_i) + U(w) \geqslant J(u) + \alpha \|u - w\|_{L^2}^2 \tag{4.10}$$

for all $\varphi_i \in \widetilde{H}^1(\Omega_w)$ and all $w \in C^{0,1}(\bar{B})$ satisfying $|\Omega_w| = |\Omega_u|$ with

$$\|w - u\|_{L^\infty(\bar{B})} \leqslant \delta, \quad \|w - u\|_{L^\infty(\bar{B})} \|\nabla(w - u)\|_{L^\infty(\bar{B})} \leqslant L. \tag{4.11}$$

In particular, there holds

$$J(w) - J(u),\ J_h(w) - J(u) \geqslant \alpha \|w - v\|_{L^2}^2$$

for all $w \in C^{0,1}(\bar{B})$ and $w \in V_h$ respectively satisfying $|\Omega_w| = |\Omega_u|$ and (4.11).

Remark 4.1. The special feature of Proposition 4.4, which is basic for the error analysis, is reflected by the fact that estimate (4.10) does not require a uniform bound of $|\nabla w|$, but, apart from the smallness of $\|w-u\|_{L^\infty}$, a bound of $\|w-u\|_{L^\infty}\|\nabla(w-u)\|_{L^\infty}$ only.

Proof. Remembering that

$$U(u+v)-U(u)+U'(u)v=\frac{1}{2}b_N\|v\|^2_{L^2}$$

and using the abbreviation

$$\Delta(\varphi,v)=Q(u+v,\varphi,f)-Q(u,f)-Q'(u,f)v,$$

it suffices to prove that if $f=f_i$, $i\in\{1,\dots,N\}$, then for any $L>0$ and $\varepsilon>0$ there exists $\delta>0$ such that

$$\Delta(\varphi,v)\geqslant\frac{1}{2}\int\limits_{\Sigma}\partial_N\big(|\nabla f|^2-|\nabla\tilde{\chi}|^2\big)v^2\,dB-\varepsilon\|v\|^2_{L^2} \tag{4.12}$$

for all $\varphi\in\widetilde{H}^1(\Omega_{u+v})$ and all $v\in C^{0,1}(\bar{B})$ with

$$\|v\|_{L^\infty(\bar{B})}\leqslant\delta,\quad \|v\|_{L^\infty(\bar{B})}\|\nabla v\|_{L^\infty(\bar{B})}\leqslant L.$$

For simplicity, we assume $\partial_N f\equiv 0$. The general case may be handled similarly but requires some additional estimates.

1^st^ Step: Transformation to Ω

Transformation to Ω gives

$$Q(u+v,\varphi,f)=\int\limits_{\Omega_{u+v}}|\nabla(\varphi+f)|^2\,dx=\int\limits_{\Omega}\sqrt{g}g^{ij}\partial_i(\psi+\chi)\partial_j(\psi+\chi)\,dx$$

with $\sqrt{g}g^{ij}$ from (2.11) and

$$\psi:=\tilde{\chi}(u+v,f)\circ\Phi(u,u+v)-\tilde{\chi}\in\widetilde{H}^1(\Omega). \tag{4.13}$$

Remembering (2.13), this implies

$$\Delta(\varphi,f)=\int\limits_{\Omega}2\nabla\chi(\partial_N\tilde{v}\nabla\psi-\nabla\tilde{v}\partial_N\psi)+(1+\partial_N\tilde{v})\left(\nabla\psi-\frac{\partial_N(\psi+\chi)}{1+\partial_N\tilde{v}}\nabla\tilde{v}\right)^2\,dx$$

after rearranging the terms. Further, noticing $\psi=0$ on Σ, $\partial_n\chi=0$ on $\Gamma\setminus\Sigma$ and $\tilde{v}=0$ on B, we get

$$\int\limits_{\Omega}\nabla\chi(\partial_N\tilde{v}\nabla\psi-\nabla\tilde{v}\partial_N\psi)\,dx=-\int\limits_{\Omega}\tilde{v}\nabla\partial_N\chi\nabla\psi\,dx$$

via integration by parts. Hence

$$\Delta(\varphi,f)=N(v,\psi)-2M(v,\psi)-P(v,\psi) \tag{4.14}$$

with the abbreviations

$$N(v,\psi) := \int\limits_{\Omega} (1+\partial_N \tilde{v}) \left(\nabla\psi - \frac{\partial_N\psi\nabla\tilde{v} + \nabla(\partial_N\chi\tilde{v})}{1+\partial_N\tilde{v}}\right)^2 dx, \tag{4.15}$$

and

$$M(v,\psi) := \int\limits_{\Omega} \frac{\partial_N\psi\nabla\partial_N\chi\tilde{v}\nabla\tilde{v}}{1+\partial_N\tilde{v}}\,dx, \quad P(v,\psi) = \int\limits_{\Omega} \frac{\nabla\big(\partial_N\chi\nabla\partial_N\chi\tilde{v}^2\big)}{1+\partial_N\tilde{v}}\,dx. \tag{4.16}$$

Note that

$$N(v,\psi) \geqslant \int\limits_{\Omega} \frac{\big(\partial_N(\psi - \partial_N\chi\tilde{v})\big)^2}{1+\partial_N\tilde{v}}\,dx \geqslant 0$$

and consequently

$$\|\psi\|^2_{L^2(\Omega)},\ \|\partial_N\psi\|^2_{L^2(\Omega)} \leqslant C\big(N(v,\psi) + \|v\|^2_{L^2(B)}\big). \tag{4.17}$$

This shows (4.12) to be valid if

$$|M(v,\psi)| \leqslant C\|v\|_{L^\infty(B)}\big(1+\|v\|_{L^\infty}\|\nabla v\|_{L^\infty}\big)\big(N(\psi,v)+\|v\|^2_{L^2}\big) \tag{4.18}$$

and

$$\left|P(v,\psi) - \frac{1}{2}\int\limits_{\Sigma} \partial_N\big(|\nabla\tilde{\chi}|^2\big)\tilde{v}^2\,dx'\right| \leqslant C\|v\|_{L^\infty(B)}\|v\|^2_{L^2(B)} \tag{4.19}$$

for every $\psi \in \widetilde{H}^1(\Omega)$ and every sufficiently small $v \in C^{0,1}(\bar{B}) : \|v\|_{C^{0,1}} < \delta$. The latter estimates will be proven in the following two steps.

2^nd^ Step: Estimation of $M(v,\psi)$

We set

$$M(v,\psi) = \int\limits_{\Omega} \partial_N\psi\,\partial_N^2\chi\,\frac{w\tilde{v}}{1+w}\,dx + \int\limits_{\Omega} \partial_N\psi\nabla\phi\nabla\rho(w)\,dx = I_1 + R_1$$

with the abbreviations

$$\rho(s) := s - \ln(1+s), \quad \phi := x_N^2\partial_N\chi, \quad w = \partial_N\tilde{v}.$$

In view of (4.17) and the uniform boundednes of $|\partial_N^2\chi|$ in Ω we get

$$|I_1| \leqslant C\|v\|_{L^\infty}\int\limits_{\Omega} |\partial_N\psi|\,|\tilde{v}|\,dx \leqslant C\|v\|_{L^\infty}\big(N(v,\psi)+\|v\|^2_{L^2}\big).$$

Integrating R_1 twice by parts shows

$$R_1 = \int\limits_{\Omega} \psi\Delta\partial_N\phi\rho(w)\,dx + \int\limits_{\Omega} \nabla\psi\nabla\partial_N\phi\rho(w)\,dx = I_2 + R_2$$

if noticing

$$\psi = 0 \text{ on } \Sigma, \quad \nabla\phi = 0 \text{ on } B, \quad \partial_n\partial_N\phi = 0 \text{ on } \Gamma\setminus\Sigma. \tag{4.20}$$

The estimate $|\rho(w)| \leqslant C|w|^2$ and the uniform bounddedness of $|\Delta\partial_N\phi|$ in Ω and (4.16) imply

$$|I_2| \leqslant C\|v\|_{L^\infty} \int_\Omega |\psi|\,|w|\,dx \leqslant C\|v\|_{L^\infty}\big(N(v,\psi) + \|v\|^2_{L^2}\big).$$

In the decomposition $R_2 = I_3 + R_3 + R_4$

$$\int_\Omega \Big(\nabla\psi - \frac{\partial_N\psi\nabla\tilde v + \nabla(\partial_N\chi\tilde v)}{1+\partial_N\tilde v}\Big)\nabla\partial_N\phi\,\rho(w)\,dx \\ + \int_\Omega \partial_N\psi\nabla\partial_N\phi\nabla\tilde v\,\frac{\rho(w)}{1+w}\,dx + \int_\Omega \nabla(\partial_N\chi\tilde v)\nabla\partial_N\phi\,\frac{\rho(w)}{1+w}\,dx,$$

I_3 can be estimated immediately through

$$|I_3| \leqslant C\|v\|_{L^\infty}\big(N(v,\psi) + \|v\|^2_{L^2}\big);$$

R_3 may be written as

$$R_3 = \int_\Omega \partial_N\psi\partial_N^2\phi\,\frac{w\rho(w)}{1+w}\,dx + \int_\Omega \partial_N\psi\nabla\phi_1\,\nabla\rho_1(w)\,dx = I_4 + R_5$$

with $\rho_1(s) = \int_0^s \rho(t)/(1+t)\,dt$ and $\phi_1 := x_N\partial_N\phi$. Then

$$|I_4| \leqslant C\|v\|^2_{L^\infty}\big(N(v,\psi) + \|v\|^2_{L^2}\big)$$

in view of (4.16). Finally, if R_4 is written as

$$R_4 = \int_\Omega \nabla(x_N\partial_N\chi)\nabla\partial_N\phi\,\frac{w\rho(w)}{1+w}\,dx + \int_\Omega x_N\partial_N\chi\nabla\partial_N\phi\nabla\rho_1(w)\,dx = I_5 + I_6,$$

we get the estimate

$$|I_5| \leqslant C\|v\|^2_{L^\infty}\|v\|^2_{L^2}.$$

Concerning I_6, we get, in view of the boundary conditions (4.20)

$$I_6 = \int_\Sigma x_N\partial_N\chi\partial_n\partial_N\phi\rho_1(w)\,dx - \int_\Omega \nabla(x_N\partial_N\chi\nabla\partial_N\phi)\rho_1(w)\,dx$$

after integrating by parts. Due to $|\rho_1(w)| \leqslant C|w|^3$ this implies

$$|I_6| \leqslant C\|v\|_{L^\infty}\|v\|^2_{L^2}.$$

It remains to estimate R_5. Since R_5 is obtained via replacing ϕ, ρ R_1 by ϕ_1, ρ_1, we get correspondingly

$$R_5 = \int_\Omega \psi\Delta\partial_N\phi_1\rho_1(w)\,dx + \int_\Omega \nabla\psi\nabla\partial_N\phi_1\rho_1(w)\,dx = I_7 + R_6$$

after integrating by parts. The uniform boundedness of $\Delta\partial_N\phi_1$ in Ω and (4.16) implies

$$|I_7| \leqslant C\|v\|^2_{L^\infty}\big(N(\psi,v)+\|v\|^2_{L^2}\big). \tag{4.21}$$

If R_6 is decomposed according to $R_6 = I_8 + I_9 + I_{10}$

$$\int_\Omega \left(\nabla\psi - \frac{\partial_N\psi\nabla\tilde{v} + \nabla(\partial_N\chi\tilde{v})}{1+\partial_N\tilde{v}}\right)\nabla\partial_N\phi_1\rho_1(w)\,dx$$
$$+\int_\Omega \partial_N\psi\nabla\tilde{v}\nabla\partial_N\phi_1\,\frac{\rho_1(w)}{1+w}\,dx + \int_\Omega \nabla(\partial_N\chi\tilde{v})\nabla\partial_N\phi_1\,\frac{\rho_1(w)}{1+w}\,dx,$$

then I_8 obeys estimate (4.21), whereas

$$|I_9| \leqslant C||\nabla v\|_{L^\infty}\|v\|^2_{L^\infty}\big(N(\psi,v)+\|v\|^2_{L^2}\big).$$

Finally, to estimate I_{10}, replace ρ,ϕ in R_4 by ρ_1,ϕ_1 to obtain

$$|I_{10}| \leqslant C\|v\|^2_{L^\infty}\|v\|^2_{L^2}.$$

This shows each integral I_k, $k=1,\dots,10$ to allow for estimate (4.18).

3rd Step: Estimation of $P(v,\psi)$

Decompose $P(v,\psi)$, after integrating by parts, according to $P(v,\psi) = I_{11} + I_{12} + I_{13}$,

$$\int_\Sigma \nabla\tilde{\chi}\nabla\partial_N\tilde{\chi}\tilde{v}^2\,dx' + \int_\Sigma \frac{\nabla\chi\nabla\partial_N\chi\partial_N\tilde{v}\tilde{v}^2}{1+\partial_N\tilde{v}}\,dx' + \int_\Omega \frac{\partial_N\chi\nabla\partial_N\chi\tilde{v}^2}{(1+\partial_N\tilde{v})^2}\nabla\partial_N\tilde{v}\,dx,$$

then I_{12} satisfies the estimate

$$|I_{12}| \leqslant C\|v\|_{L^\infty(B)}\|v\|^2_{L^2(B)}.$$

If we set $w=\partial_N\tilde{v}$ and $\rho_2(s) = \int_0^s t^2(1+t)^{-2}\,dt$, the last term can be written as

$$I_{13} = \int_\Omega x_N^2\partial_N\chi\nabla\partial_N\chi\nabla\rho_2(w)\,dx.$$

Now, integration by parts leads to

$$I_{13} = \int_\Sigma x_N^2\partial_N\chi\partial_N^2\chi\rho_2(w)\,dB - \int_\Omega \nabla(x_N^2\partial_N\chi)\partial_N^2\chi\rho_2(w)\,dx,$$

hence

$$|I_{13}| \leqslant C\|v\|_{L^\infty(B)}\|v\|^2_{L^2(B)}$$

in view of $|\rho_2(w)| \leqslant C|w|^3$ and $|\nabla\partial_N\chi| \leqslant C$ in $\Omega\cup\Sigma$. Thus, $|P-I_{11}|$ satisfies estimate (4.19).

□

Proposition 4.5. *Let $\tilde{u}_h = \pi_h^B u + const \in V_h$ with a constant that guarantees the volume constraint $|\Omega| = |\Omega_{u_h}|$. If $N = 2, 3$ and $m \geqslant 2$, then there exists $C > 0$ with the property*

$$J_h(\tilde{u}_h) \leqslant J(u) + Ch^3 \quad \textit{for all } h > 0.$$

If $N = 2$ and $m = 1$, the exponent is to be replaced by h^2.

Proof. We restrict the proof to the 3D case. For shortness we set $\Omega_h = \Omega_{\tilde{u}_h}$, $\widetilde{W}_h = \widetilde{W}_h^{\tilde{u}_h}$, $\Pi_h = \Pi_h^{\tilde{u}_h}$. The letter C always indicates a constant independent of h. Due to (4.1) we have

$$\|u - \tilde{u}_h\|_{L^\infty(B)} + h\|u - \tilde{u}_h\|_{W^{1,\infty}(B)} \leqslant Ch^2,$$

hence

$$|U(\tilde{u}_h) - U(u) - U'(u)(\tilde{u}_h - u)| = \frac{1}{2} b_3 \|u - \tilde{u}_h\|^2_{L^2(B)} \leqslant Ch^4,$$

in particular. Thus, it suffices to prove that for any $f = f_i$, $i = 1, 2, 3$, there exists $\varphi \in W_h$ such that

$$|\Delta_h(\varphi)| := |Q(\tilde{u}_h, \varphi, f) - Q(u, f) - Q'(u, f)(u - \tilde{u}_h)| \leqslant Ch^3.$$

Remembering (4.14) and estimates (4.18), (4.19), we infer the existence of $\delta > 0$ such that for all $v \in C^{0,1}(\bar{B})$ with $\|v\|_{C^{0,1}} \leqslant \delta$ there holds

$$|Q(u + v, \varphi, f) - Q(u, f) - Q'(u, f)v| \leqslant C\big(N(v, \psi) + \|v\|^2_{L^2}\big),$$

where ψ and $N(v, \psi)$ are defined by (4.13) and (4.15) respectively. Moreover,

$$N(v, \psi) \leqslant 2 \int\limits_{\Omega} \big|\nabla(\psi - \partial_3 \chi \tilde{v})\big|^2 \, dx + C\|v\|_{W^{1,\infty}} \big(\|\partial_3 \psi\|^2_{L^2} + \|v\|^2_{L^2}\big)$$

by (4.15), which implies

$$N(v, \psi) \leqslant C\Big(\int\limits_{\Omega} \big|\nabla(\psi - \partial_3 \chi \tilde{v})\big|^2 \, dx + \|v\|^2_{L^2}\Big)$$

in view of (4.17), provided $\delta > 0$ is sufficiently small. Thus, there exists $h_0 > 0$ with the property

$$|\Delta_h(\varphi)| \leqslant C\Big(\int\limits_{\Omega} \big|\nabla(\psi - \partial_3 \chi \tilde{v}_h)\big|^2 \, dx + h^4\Big)$$

for $0 < h < h_0$ and $\varphi \in \widetilde{H}^1(\Omega_h)$, where we have set $v_h := \tilde{u}_h - u$. After transformation to Ω_h this estimate can be written as

$$|\Delta_h(\varphi)| \leqslant C\Big(\int\limits_{\Omega_h} \big|\nabla(\varphi - \phi_1 - \phi_2)\big|^2 \, dx + h^4\Big),$$

where we have set

$$\phi_1(x', x_N) = \tilde{\chi}\big(x', x_N u(x')/\tilde{u}_h(x')\big),$$
$$\phi_2(x', x_N) = \partial_N \chi\big(x', x_N u(x')/\tilde{u}_h(x')\big) x_N \big(u(x') - \tilde{u}_h(x')\big)/\tilde{u}_h(x').$$

Hence it remains to prove

$$\min\left\{\|\nabla(\varphi-\phi_i)\|^2_{L^2(\Omega_h)} \mid \varphi\in\widetilde{W}_h\right\}\leqslant Ch^3,\quad i=1,2. \tag{4.22}$$

The function $\tilde{u}_h(x')$ being an affine one of its arguments if $(x',x_N)\in T$, $T\in\mathscr{T}_h^{\tilde{u}_h}$, we have

$$\|\phi_1\|_{W^{3,\infty}(T)}\leqslant C \text{ for all } T\in\mathscr{T}_h^{\tilde{u}_h}$$

since $\|\Phi(\tilde{u}_h,u)|_T\|_{W^{3,\infty}(T)}\leqslant C$. Consequently, by (4.4)

$$\left\|\nabla(\Pi_h\phi_1-\phi_1)\right\|^2_{L^2(T)}\leqslant C|T|h^4,$$

which shows (4.22) for $i=1$.

To treat the case $i=2$, we choose cut-off functions $\rho_h\in C^3(\Omega_h)$, $0\leqslant\rho_h\leqslant 1$ such that

$$\rho_h=\begin{cases}1 & \text{in } \Omega'_h:=\Omega_{\tilde{u}_h-2h},\\ 0 & \text{in } \Omega_h\setminus\Omega_{\tilde{u}_h-h},\end{cases}$$

and

$$\|\rho_h\|_{W^{l,\infty}(\Omega_h)}\leqslant Ch^{-l},\quad l=1,2,3.$$

Then $\rho_h\phi_2\in\widetilde{H}^1(\Omega_h)$ and

$$\|\varrho\phi_2\|_{W^{3,\infty}(T)}\leqslant\begin{cases}C & \text{if } T\in\mathscr{J}:=\{T\in\mathscr{T}_h^{\tilde{u}_h}\mid T\subseteq\Omega'_h\},\\ Ch^{-1} & \text{if } T\in\mathscr{I}:=\mathscr{T}_h^{\tilde{u}_h}\setminus\mathscr{J},\end{cases}$$

if $u\in W^{3,\infty}(B)$ is remembered. This implies, as above,

$$\|\nabla\left(\Pi_h(\varrho\phi_2)-\varrho\phi_2\right)\|^2_{L^2(T)}\leqslant\begin{cases}C|T|h^4 & \text{if } T\in\mathscr{J},\\ C|T|h^2 & \text{if } T\in\mathscr{I},\end{cases}$$

in view of (4.4). Hence

$$\left\|\nabla\big(\Pi_h(\rho\phi_2)-\rho\phi_2\big)\right\|^2_{L^2(\Omega_h)}\leqslant\sum_{T\in\mathscr{J}}C|T|h^4+\sum_{T\in\mathscr{I}}C|T|h^2\leqslant Ch^3.$$

Because of

$$\left|\nabla\big((1-\rho_h)\phi_2\big)\right|\leqslant|\nabla\phi_2|+Ch^{-1}|\phi_2|\leqslant Ch,$$

we obtain finally

$$\left\|\nabla\big((1-\rho_h)\phi_2\big)\right\|^2_{L^2(\Omega_h)}=\left\|\nabla\big((1-\rho_h)\phi_2\big)\right\|^2_{L^2(\Omega_h\setminus\Omega'_h)}\leqslant Ch^3,$$

which completes the proof. □

Proof of Theorem 4.3. Setting

$$K_h=\left\{v_h\in V_h\;\Big|\;\|v_h-u\|_{L^2(\bar{B})}\leqslant\beta h^{3/2},\ |\Omega|=|\Omega_{u_h}|\right\}$$

with a sufficiently large $\beta>0$ to be chosen later, we have in view of the inverse estimates (4.2)

$$\|u-v_h\|_{L^\infty(\bar{B})}\leqslant C\beta h^{1/2},\quad \|u-v_h\|_{L^\infty(\bar{B})}\|\nabla(u-v_h)\|_{L^\infty(\bar{B})}\leqslant C\beta^2$$

for all $v_h \in K_h$ with C independent of β. By Proposition 4.4 there exist $\alpha > 0$ and $h_0 = h_0(\beta) > 0$ such that

$$J_h(v_h) - J(u) \geqslant \alpha \|u - v_h\|^2_{L^2(\bar{B})} \tag{4.23}$$

for all $v_h \in K_h$ with $0 < h < h_0$. Since Proposition 4.5 guarantees

$$J(u_h) \leqslant J(u) + \gamma h^3,$$

for any minimizer $u_h \in K_h$ of $J_h \to \min_{v_h \in K_h}$, estimate (4.23) implies

$$\|u - u_h\|_{L^2(\bar{B})} \leqslant \beta h^{3/2}/2$$

if $\beta > 2\sqrt{\gamma/\alpha}$. This shows u_h to belong to the interior of K_h. □

5. Numerical examples

In this section we present some results of our numerical tests. As mentioned in the introduction, we restrict ourselves to the determination of local minimizers to the discretized effective potential (4.6). The figures below show the behaviour of the minimizing free surface for various values of gravity, vibration and volume relative to different geometric configurations. For some ranges of the parameters the computational results are in good agreement with experimental data (cf. [8, 11, 21]), whereas configurations similar to Fig. 7 seem to be of less physical significance. Our computation uses standard methods for optimal shape design problems: conjugate gradient method combined with a line search method. Since the computation of the discretized gradient (4.9) requires no essential additional effort, the line search based on the quadratic fitting turned out to be sufficient for our purposes. All tests led to the independence of the minimizer of the arbitrarily chosen initial shapes as long as the initial surface remains bounded away from the bottom. The grid generation adopts essentially the lines described in Section 4, i.e., independently of the actual geometric configuration free boundary and flow domain are related by an appropriate correspondence. We made use of linear elements together with 101×101 and $25 \times 25 \times 25$ grid points for 2D and 3D flows, respectively. To get a stopping criterion, the L^∞-norm of the discretized gradient was required to be less than 10^{-5}.

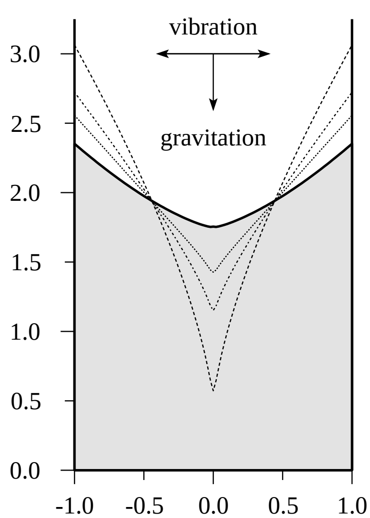

Figure 1. $b_2 = 4.0, 1.5, 0.8, 0.3$

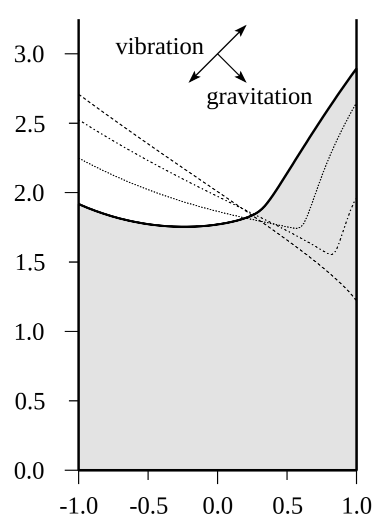

Figure 2. $b_1 = 4.5, 2.0, 1.0, 0.5$

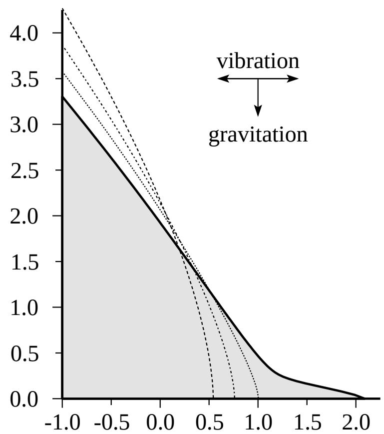

Figure 3. $b_2 = 0.5, 0.4, 0.3, 0.2$

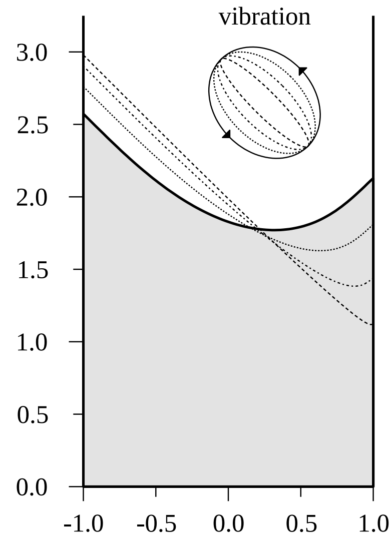

Figure 4. $\mu = 0.8, 0.6, 0.4, 0.2$

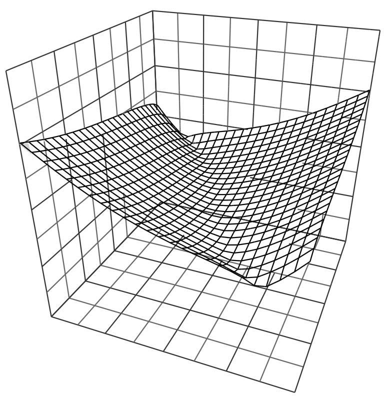

Figure 5. $f_1 = 2x_1 + x_2$, $b_1 = b_2 = 0.0$, $b_3 = 20.0$, $vol = 4.0$

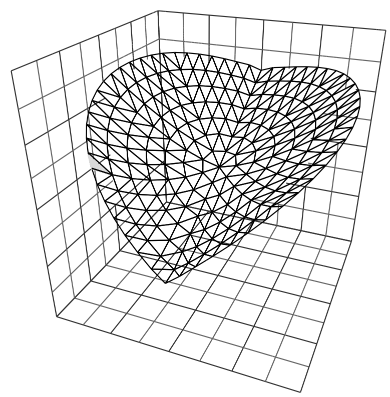

Figure 6. $f_1 = x_1$, $b_1 = 0.0$, $b_2 = -2.5$, $b_2 = 5.0$, $vol = 4.0$

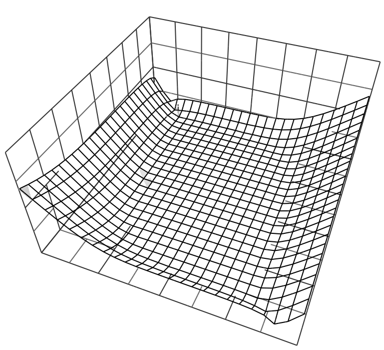

Figure 7. $f_1 = 2x_1 + x_2$, $b_1 = b_2 = 0.0$, $b_3 = 20.0$, $vol = 0.8$

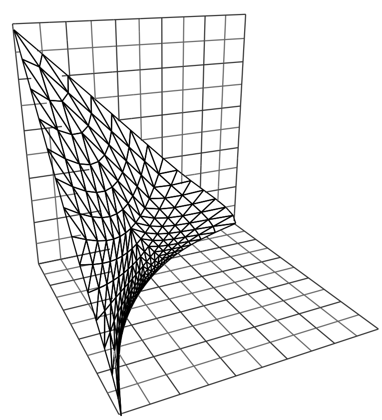

Figure 8. $f_1 = x_1 + x_2$, $b_1 = b_2 = 0.0$, $b_3 = 1.0$, $vol = 2.0$

In 2D, Fig. 1 illustrates the simplest situation of a horizontal vibration of a rectangular container in a vertical gravity field, i.e., $f_1 = x_1$, $f_2 \equiv 0$ and $b_1 = 0, b_2 > 0.0$ in (2.6), (2.1). The total volume is normed by 4.0, which corresponds to a planar horizontal equilibrium surface with height 2.0 in a pure gravity field. The dotted lines show the behaviour of the free boundary under a decreasing gravity. The numerical results indicate that the originally smooth free boundary develops a cusp on the symmetry axis which, for the limiting value of b_2, eventually touches the bottom. For lower values of b_2 the fluid divides into two separated portions. Fig. 3 shows the typical shape of the left part (with volume 4.0) of the fluid which is separated this way. Fig. 2 shows the minimizer in an oblique container: $f_1 = x_1 + x_2$, $b_2 = -b_1$. Finally, Fig. 4 refers to the case of an 'elliptic' vibration: $f_1 = x_1 + x_2, f_2 = \mu(x_1 - x_2)$ in zero gravity. For similar tests in 2D using boundary integral methods we refer the reader to [9].

In 3D, Figs. 5-8 show some typical shapes of the optimal free surface. To get an impression of the height, relations grid lines (distance 0.25) have been added.

Figs. 5 and 7 relate to a fluid in a cylinder with square cross section (side length 2.0) subject to a vertical gravitational field and a horizontal vibration, whereas Fig. 6 refers to an oblique circular cylinder (diameter 2.0). Fig. 8 illustrates the case where a part of the fluid is separated in a corner of the container which is the 3D analogue of the situation shown in Fig. 3.

References

[1] T. B. Benjamin and F. Ursell, *The Stability of the Plane Free Surface of a Liquid in Vertical Periodic Motion*, Proc. Royal Soc. London, Ser. A, Math. Phys., **225** (1954), pp. 505–515.

[2] K. Beyer, I. Gawriljuk, M. Günther, I. Lukowsky, and A. Timokha, *Compressible potential flows with free boundaries. Part I: Vibrocapillary Equilibria*, Z. Angew. Math. Mech., **81** (2001), No. 4, pp. 261–271.

[3] I. Blekhman, *Vibrational Mechanics*, World Scientific, Singapore, 1999.

[4] N. N. Bogoljubow and J. A. Mitropolski, *Asymptotische Methoden in der Theorie der nichtlinearen Schwingungen*, Akademie-Verlag, Berlin, 1965.

[5] S. C. Brenner and L. R. Scott, *The Mathematical Theory of Finite Element Methods*, Springer Verlag, New York, 1994.

[6] D. Cioranescu and P. Donato, *An Introduction to Homogenization*, Oxford University Press, Oxford, 1999.

[7] M. Faraday, *On a peculiar class of Acoustical Figures*, Phil. Trans. Royal Soc. London, **52** (1831), pp. 209–340.

[8] R. F. Ganiyev, V. D. Lakiza, and A. S. Tsapenko, *On dynamic behaviour of a free liquid surface under low gravity and vibrational effects.*, Prikladnaya Mekhanika (Soviet Applied Mechanics) **13** (1977), No. 5, pp. 102–107, in Russian.

[9] I. Gavrilyuk, I. Lukovsky, and A. Timokha, *Two-Dimensional Vibroequilibria and Faraday's Drops*, to appear in ZAMP.

[10] J. Haslinger and P. Neittaanmäki, *Finite Element Approximation for Optimal Shape Design*, John Wiley, Chichester, 1988.

[11] A. A. Ivanova, V. G. Kozlov, and S. I. Tashkinov, *Interface dynamics of immiscible fluids under circularly polarized vibration (experiment)*, Fluid Dynamics, **36** (2001), No. 6, pp. 871–879, translated from Izvestiya Rossiiskoi Academii Nauk, Mekhanika Zhidkosti i Gaza.

[12] P. L. Kapitsa, *The pendulum with a vibrating suspension*, Uspechi Fiz. Nauk **44** (1951) No. 1, pp. 7–20, in Russian.

[13] T. Kato, *Locally coercive nonlinear equations, with applications to some periodic solutions*, Duke Math. J., **51** (1984), pp. 923–936.

[14] L. D. Landau and E. M. Lifschitz, *Lehrbuch der theoretischen Physik I: Mechanik*, Akademie-Verlag, Berlin, 1976.

[15] M. Levi, *Geometry and physics of averaging with applications*, Physica D, **132** (1999), No. 1–2, pp. 150–164.

[16] W. Paul, *Electromagnetic traps for charged and neutral particles*, Rev. Mod. Phys., **62** (1990), pp. 531–540.

[17] O. Pironneau, *Optimal Shape Design for Elliptic Systems*, Springer Verlag, New York, 1984.

[18] J. A. Sanders and F. Verhulst, *Averaging methods in nonlinear dynamical systems*, Springer Verlag, New York, 1985.

[19] J. Sokolowski and J.-P. Zolesio, *Introduction to Shape Optimization*, Springer Verlag, Berlin, 1992.

[20] A. Timokha, *The behaviour of a free liquid surface in a vibrating container*, Prepr. 92.22, Inst. Math. Acad. Sci. Ukraine, Kiev, 1992, in Russian.

[21] G. H. Wolf, *Dynamic stabilisation of the interchange instability of a liquid-gas interface*, Phys. Rev. Lett., **24** (1970), No. 9, pp.444–446.

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