

Computation of free surfaces in the electromagnetic shaping of liquid metals by optimization algorithms

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ABSTRACT. — We describe a numerical method to compute free surfaces in the electromagnetic shaping of liquid metals. It is based on an energetic variational formulation for the equilibrium so that optimization algorithms of a quasi-Newton type are used like the so-called BFGS method. The elliptic problem in an exterior domain involved in the computation of the gradient with respect to the domain at each step is solved by a boundary integral representation. Several examples are given for the case of a vertical column of molten metal.

1. Introduction

There are several engineering processes where the free surface of a molten metal is shaped by electromagnetic forces. The control of these surfaces leads to various mathematical questions and requires numerical simulation. Often the computation of the free boundary amounts to solving an "optimal design" problem where the functional to be optimized is the total energy of the phenomenon under consideration. As such the numerical question is very general and has a wide range of applications. Therefore it is of interest to develop corresponding algorithms of a general nature.

Our goal here is to develop numerical methods to compute the free surfaces in the electromagnetic shaping of molten metals by optimization techniques. Although our approach extends to 3-dimensional situations, we will restrict ourselves to a 2-dimensional model since its actual 3-*d* implementation is still in progress. It concerns the case of a vertical column of liquid metal falling down in an electromagnetic field created by vertical conductors. We assume the frequency of the imposed current is very high so that the magnetic field does not penetrate into the metal and the electromagnetic forces are reduced to the magnetic pressure acting on the interface. Moreover, we assume that a stationary horizontal section is reached so that the following simple 2-dimensional model is valid.

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We denote by Ω the exterior in the plane of the closed and simply connected domain occupied by the metal. We deal with the mean square values of the relevant quantities: $\mathbf{j}_0 = (0, 0, j_0)$ denotes the density current vector, $\mathbf{B} = (B_1, B_2, 0)$ is the total magnetic field. We have the following system of equilibrium:

$$(1.1) \quad \nabla \wedge \mathbf{B} = \mu_0 \mathbf{j}_0 \quad \text{in } \Omega,$$

$$(1.2) \quad \nabla \cdot \mathbf{B} = 0 \quad \text{in } \Omega,$$

$$(1.3) \quad \mathbf{B} \cdot \mathbf{n} = 0 \quad \text{on } \Gamma = \partial\Omega,$$

$$(1.4) \quad |\mathbf{B}|^2 / 2\mu_0 + \sigma \mathcal{C} = \text{constant on } \Gamma,$$

$$(1.5) \quad |\mathbf{B}| = O(|x|^{-2}) \quad \text{as } |x| \rightarrow \infty \quad \text{in } \Omega,$$

where μ_0 is the vacuum permeability, \mathbf{n} the unit normal vector to the boundary Γ , \mathcal{C} the curvature of Γ (seen from the metal), σ the surface tension of the liquid and $|\cdot|$ denotes the euclidian norm. The constant in (1.4) is an unknown of the problem. Obviously the boundary Γ is also unknown.

This problem or very similar ones have been considered in several places in the literature. We refer the reader to the following papers and to references in them for the physical analysis of the simplifying assumptions that the above model requires: see ([Shercliff, 1981]; [Sero-Guillaume, 1983]; [Brancher & Sero-Guillaume, 1983]; [Sneyd & Moffatt, 1982]; [Brancher *et al.*, 1983]; [Gagnoud *et al.*, 1986]; [Mestel, 1982]; [Etay *et al.*, 1988]).

Our purpose is to describe an algorithm to compute the free boundary Γ based on an equivalent variational formulation of (1.1)-(1.5) involving the total energy. This kind of equivalence can be found in several places in the literature since Bernoulli conditions like (1.4) often appear in hydrodynamic problems and various fluid problems; let us refer for instance to [S, 1983] where a large class of liquid metal equilibria is considered and also [Zolésio, 1983] for fluid problems and [Zolésio, 1990] for a survey with many references.

Numerical computations of shapes in particular situations and with different methods can also be found in ([S, 1981]; [Gagnoud & Sero-Guillaume, 1986]; [Coulaud & Henrot, 1990]; [Etay, 1982]; [Li & Evans, 1989]). Our approach here is very general and allows us to handle any kind of distribution j_0 and any value of the surface tension. This flexibility arises from the choice of sophisticated optimization algorithms which, in particular, do not require any *a priori* symmetry assumption on the data. Moreover, the method carries over to other problems (see e. g. Sec. 5).

2. The variational formulation

Conditions (1.2), (1.3) imply that $\mathbf{B} = (\varphi_y, -\varphi_x, 0)$ where $\varphi : \Omega \rightarrow \mathbf{R}$. The total energy can be written in terms of φ and Ω as

$$(2.1) \quad E(\Omega) = -\frac{1}{2\mu_0} \int_{\Omega} |\nabla \varphi|^2 + \sigma P(\Omega)$$

where $P(\Omega)$ is the perimeter of Ω , *i.e.* the length of $\partial\Omega$ when $\partial\Omega$ is regular enough (for instance of class C^1) and can be written as

$$P(\Omega) = \int_{\partial\Omega} d\Gamma, \quad d\Gamma = \text{length measure on } \Gamma = \partial\Omega,$$

and φ is the solution of (see (1.1), (1.3), (1.5))

$$(2.2) \quad -\Delta\varphi = \mu_0 j_0 \quad \text{in } \Omega,$$

$$(2.3) \quad \varphi = 0 \quad \text{on } \Gamma,$$

$$(2.4) \quad \varphi(x) = O(|x|^{-1}) \quad \text{as } |x| \rightarrow \infty.$$

Condition (1.3) implies that φ is constant on Γ ; we normalize it to zero.

The variational formulation of (1.1)-(1.5) consists of considering the equilibrium domain Ω as a stationary point for the functional (2.1), where Ω is the variable, under the constraint that $m(\complement\Omega)$ be imposed ($\complement\Omega$ = complement of Ω , m = Lebesgue measure in \mathbb{R}^2). This point of view is summarized next.

THEOREM 2.1. — *Let Ω be the complement of a compact set in \mathbb{R}^2 with nonempty interior. Assume that $\partial\Omega$ is of class C^2 . Let V be in $C^1(\mathbb{R}^2, \mathbb{R}^2)$ with compact support and*

$$(2.5) \quad \forall x \in \mathbb{R}^2, \quad T_t x = x + tV(x),$$

$$(2.6) \quad \Omega_t = T_t(\Omega), \quad \partial\Omega_t = T_t(\partial\Omega) \quad (t \text{ small enough}).$$

Finally let j_0 be a square integrable function from Ω into \mathbb{R} with compact support in Ω .

Then, for t small enough, there exists a unique solution $\varphi(x, t)$ of

$$(2.7) \quad -\Delta_x \varphi(x, t) = \mu_0 j_0(x) \quad \text{in } \Omega_t,$$

$$(2.8) \quad \varphi(x, t) = 0 \quad \text{on } \partial\Omega_t, \quad \varphi(t) = O(|x|^{-1}) \quad \text{as } |x| \rightarrow \infty.$$

Moreover, if

$$(2.9) \quad E(\Omega_t) = -\frac{1}{2\mu_0} \int_{\Omega} |\nabla \varphi(x, t)|^2 dx + \sigma P(\Omega_t),$$

then for all $P_0 \in \mathbb{R}$:

$$(2.10) \quad \frac{d}{dt} (E(\Omega_t) - P_0 m(\Omega_t))|_{t=0} = \int_{\partial\Omega} \left(\frac{1}{2\mu_0} |\nabla \varphi|^2 + \sigma \mathcal{E} - P_0 \right) V \cdot n$$

where n is the unit normal derivative to $\partial\Omega$ oriented towards Ω .

Remark

Differentiation with respect to the domain is classical in the literature. Very similar results can be found for instance in the above mentioned papers ([S, 1989]; [Z, 1984]. See also [Descloux, 1990]). A complete proof under precisely the above regularity assumptions is given in [Pierre & Roche, 1990]. It is not reproduced here. Definitions and

relevant results concerning regularity of boundaries (such as the notion of class C^2) can be found in [Grisvard, 1985]. The function $\varphi(\cdot, t)$ has locally square integrable second derivatives so that (2.7) can be understood in the L^2 -sense. Moreover, the traces of φ and $\nabla \varphi$ on $\partial\Omega$ exist and are (at least) square integrable on $\partial\Omega$.

According to (2.10) the variational formulation of the continuous problem (1.1)-(1.5) consists of finding (Ω, P_0) such that

$$(2.11) \quad \frac{d}{dt} (E(\Omega_t) - P_0 m(\Omega_t)) \Big|_{t=0} = 0.$$

Note that computing this derivative for a given Ω requires the solution of a boundary value problem in an exterior domain. This makes the numerical approach highly non-trivial.

3. The discretization and the algorithm

The discretization consists of constructing a sequence (Γ^k, ψ^k, Z^k) where Γ^k is a piecewise linear closed Jordan curve, ψ^k is an approximation of the solution of

$$(3.1) \quad -\Delta \varphi^k = \mu_0 j_0 \quad \text{on } \Omega^k = \text{exterior of } \Gamma^k,$$

$$(3.2) \quad \varphi^k|_{\Gamma} = 0, \quad \varphi^k(x) = O(|x|^{-1}) \quad \text{as } |x| \rightarrow \infty,$$

and Z^k is a vector field defining the direction of displacement of the nodes of Γ^k .

These are moved according to a perturbed gradient algorithm for the *penalized mapping*:

$$(3.3) \quad \Omega \mapsto E_\mu(\Omega) = E(\Omega) + \mu(m(\Omega) - S_0)^2,$$

where S_0 is the prescribed area and μ a positive number, large enough so that the solution Ω satisfies the constraint $m(\Omega) = S_0$ as well as possible.

Let us introduce some notation. By Γ^k , we mean the piecewise linear Jordan curve with n edges $[x_i^k, x_{i+1}^k]$, $i = 1, \dots, n$ and $x_{n+1}^k = x_1^k$. With Γ^k is associated a vector field $Z^k = (Z_i^k)_{i=1, \dots, n}$ and for $u \in \mathbb{R}^n$, we denote by Γ_u^k the perturbed curve whose vertices are

$$(3.4) \quad \{x_i^k + u_i Z_i^k; i = 1, \dots, n\} \quad (\text{definition of } \Gamma_u^k).$$

We denote by Ω_u^k the exterior of Γ_u^k . The corresponding energy is defined as

$$(3.5) \quad E_\mu^k(u) = -\frac{1}{2\mu_0} \int_{\Omega_u^k} |\nabla \varphi_u^k|^2 + \sigma P(\Omega_u^k) + \mu(m(\Omega_u^k) - S_0)^2$$

where φ_u^k is the solution of

$$(3.6) \quad \begin{cases} -\Delta \varphi_u^k = \mu_0 j_0 & \text{in } \Omega_u^k, \\ \varphi_u^k = 0 & \text{on } \Gamma_u^k, \varphi_u^k(x) = O(|x|^{-1}) \quad \text{as } |x| \rightarrow \infty. \end{cases}$$

Similarly to (2.10), we have a formula for the gradient of the above discretized energy (see [P & R, 1990] for a detailed proof). Here we write φ^k for φ_0^k and Ω^k for Ω_0^k .

PROPOSITION 3.1. — *Under the above assumptions*

$$(3.7) \quad \frac{\partial}{\partial u_i} E_\mu^k(u)|_{u_i=0} = \frac{1}{2\mu_0} \int_{\Gamma^k} |\nabla \varphi^k|^2 (\tilde{Z}_i^k \cdot n) d\Gamma^k \\ + \sigma \left(\frac{x_i^k - x_{i-1}^k}{|x_i^k - x_{i-1}^k|} - \frac{x_{i+1}^k - x_i^k}{|x_{i+1}^k - x_i^k|} \right) \cdot Z_i^k + 2\mu (m({}^c\Omega^k) - S_0) \int_{\Gamma^k} (\tilde{Z}_i^k \cdot n) d\Gamma^k$$

where \tilde{Z}_i^k is the piecewise linear vector field on Γ^k such that

$$(3.8) \quad \tilde{Z}_i^k(x_j^k) = 0 \quad \text{if } j \neq i, \quad \tilde{Z}_i^k(x_i^k) = Z_i^k.$$

Remark

Note that \tilde{Z}_i^k is supported by $[x_{i-1}^k, x_i^k] \cup [x_i^k, x_{i+1}^k]$, so that the above integrals on Γ^k can be replaced by integrals on $[x_{i-1}^k, x_i^k] \cup [x_i^k, x_{i+1}^k]$.

A pure gradient algorithm would now consist in setting

$$(3.9) \quad \Gamma^{k+1} = \Gamma_{u^k}^k,$$

where, for an appropriately chosen $\rho > 0$:

$$(3.10) \quad u_i^k = -\rho \frac{\partial}{\partial u_i} E_\mu^k|_{u_i=0}, \quad i = 1, \dots, n.$$

We modify this in two ways. First the gradient is not exactly computed as in (3.7). Indeed, it would require the knowledge of the exact solution φ^k of (3.6) at $u=0$. This problem is itself discretized and an approximate solution ψ^k of φ^k is computed as indicated in the next section. The gradient is modified accordingly: since $|\nabla \varphi^k| = (\nabla \varphi^k \cdot n)$ on Γ^k , it is natural to replace (3.7) by

$$(3.11) \quad D_i E_\mu^k = \frac{1}{2\mu_0} \int_{\Gamma^k} (\nabla \psi^k \cdot n)^2 (\tilde{Z}_i^k \cdot n) d\Gamma^k + \sigma \left(\frac{x_i^k - x_{i-1}^k}{|x_i^k - x_{i-1}^k|} - \frac{x_{i+1}^k - x_i^k}{|x_{i+1}^k - x_i^k|} \right) \cdot Z_i^k \\ + 2\mu (m({}^c\Omega^k) - S_0) \int_{\Gamma^k} (\tilde{Z}_i^k \cdot n) d\Gamma^k.$$

We denote by DE_μ^k the vector with components $D_i E_\mu^k$, $i = 1, \dots, n$.

Next, the gradient algorithm with constant path turns out to be rather slow. Consequently, a more efficient method is chosen, namely the so-called BFGS quasi-Newton algorithm named after its authors Broyden, Fletcher, Goldfarb, Shanno who independently introduced it at about the same time (1969-1970) (see for instance [Minoux, 1983] for details about it). For this we choose intermediate steps $k_1 < k_2 < \dots < k_p < \dots$

Then for all $p \geq 1$ we fix $\rho_p \in (0, 1]$, $Z^p \in (\mathbb{R}^2)^n$ and we set

$$(3.12) \quad H^{k_p} = \text{Identity in } \mathbb{R}^n, \quad Z^{k_p} = Z^p.$$

For $k = k_p$ to $k_{p+1} - 1$:

$$(3.13) \quad u^k = -\rho_p H^k DE_\mu^k [\text{see (3.11)}],$$

$$(3.14) \quad \Gamma^{k+1} = \Gamma_{u^k}^k, \quad Z^{k+1} = Z^k,$$

$$(3.15) \quad \gamma^k = DE_\mu^{k+1} - DE_\mu^k,$$

$$(3.16) \quad H^{k+1} = H^k + \left[1 + \frac{g^k H^k \gamma^k}{v^k \gamma^k} \right] \frac{u^k v^k}{v^k \gamma^k} - \frac{u^k g^k H^k + H^k \gamma^k v^k}{v^k \gamma^k},$$

where $g^k = {}^t \gamma^k =$ transpose of γ^k , $v^k = {}^t u^k$.

Remark

The main property of this algorithm is that, under suitable assumptions, the matrices H^k "converge" to $(\nabla_\mu^2 E)^{-1}$ and (3.12)-(3.16) is now almost the usual Newton's method.

Note that the field of displacement is kept constant from k_p to k_{p+1} [see (3.14)]. It is renewed each time [see (3.12)]. In actual computations, various choices have been made for Z^p such as:

- $Z^p = Z^1 =$ constant for star-shaped domains;
- $Z^p =$ approximate normal to Γ^{k_p} (Z_i^p bisecting the angle of the i -th vertex). Different choices for Z^p do not seem to change the computed equilibrium shapes as long as they reasonably "fit" their geometry. This is consistent with the fact that displacements of continuous curves can be similarly represented by $x \mapsto x + u(x)Z(x)$ where Z is any reasonable field. We have also included the possibility of progressively increasing the number of points: this allows the acceleration of the first few iterations (by starting with less points) and also adds more points in the regions where they are needed.

4. Computation of the approximate solution ψ^k

A knowledge of ψ^k is necessary for the computation of the approximate gradient of E_μ . As shown by (3.11), we actually only need to know $\nabla \psi^k$ at the boundary. Therefore, it is natural to choose a *boundary integral representation* for ψ^k .

For this, we first introduce the function

$$(4.1) \quad \theta(x) = -\frac{\mu_0}{2\pi} \int_{\mathbb{R}^2} \ln|x-y| j_0(y) dy + \frac{\mu_0}{2\pi} \ln|x| \int_{\mathbb{R}^2} j_0(y) dy.$$

Since

$$(4.2) \quad -\Delta\theta = \mu_0 j_0 \text{ in } \mathbb{R}^2, \quad \theta(x) = O(|x|^{-1}) \text{ as } |x| \rightarrow \infty,$$

the problem (3.6) with $u=0$ is equivalent to:

$$(4.3) \quad \varphi^k = \theta^k + \theta,$$

$$(4.4) \quad -\Delta \theta^k = 0 \quad \text{in } \Omega_\mu^k,$$

$$(4.5) \quad \theta^k = -\theta \quad \text{on } \Gamma^k,$$

$$(4.6) \quad \theta^k(x) = O(|x|^{-1}) \quad \text{as } |x| \rightarrow \infty.$$

Note that the second term in the definition of θ is needed for (4.6) to hold. It is well-known (see e. g. [Nedelec, 1977]) that θ^k can be represented by

$$(4.7) \quad \forall x \in \Omega^k \cup \Gamma^k, \quad \theta^k(x) = -\frac{1}{2\pi} \int_{\Gamma^k} q(y) \ln|x-y| dy,$$

where the unknown function q is defined implicitly by the system (4.5), (4.7). This system is discretized using a finite element representation for the approximation q^k of q . We introduce the basis $\{e_j^k\}_{j=1, \dots, n}$ where e_j^k is piecewise constant on Γ^k and defined by

$$(4.8) \quad \forall i, j=1, \dots, n: \quad e_j^k(x) = \begin{cases} 1 & \text{if } x \in [x_i, x_{i+1}]. \\ 0 & \text{otherwise.} \end{cases}$$

Then, q^k is obtained as $q^k = \sum_{j=1}^n \eta_j^k e_j^k$ where $(\eta_j^k)_{j=1, \dots, n} \in \mathbb{R}^n$ is solution of the discretized version of (4.5), (4.7), namely

$$(4.9) \quad \int_{\Gamma^k} e_i^k(x) \left\{ \frac{1}{2\pi} \int_{\Gamma^k} q^k(y) \ln|x-y| dy \right\} dx = \int_{\Gamma^k} e_i^k(x) \theta(x) dx, \quad i=1, \dots, n.$$

This is a $n \times n$ linear system with matrix $A^k = [a_{ij}^k]_{i,j=1, \dots, n}$ where

$$(4.10) \quad a_{ij}^k = \frac{1}{2\pi} \int_{\Gamma^k \times \Gamma^k} e_i^k(x) e_j^k(y) \ln|x-y| dx dy.$$

Once q^k is obtained, the approximate solution $\tilde{\theta}^k$ of θ^k is given by formula (4.7) with q replaced by q^k and θ^k by $\tilde{\theta}^k$. Actually, only the gradient of $\tilde{\theta}^k$ on Γ^k is needed. Indeed, the approximate gradient DE_μ^k is computed according to (3.11) where

$$\nabla \psi^k \cdot n = \nabla \theta \cdot n + \nabla \tilde{\theta}^k \cdot n$$

and [see (4.7)]

$$\nabla \tilde{\theta}^k \cdot n = -\frac{1}{2\pi} \int_{\Gamma^k} q^k(y) \nabla_x (\ln|x-y|) \cdot n dy.$$

Important remark

Actual computations will be made for given current densities j_0 which are the sum of Dirac masses (case of vertical wires). It is well-known that the total energy is then

unbounded. Nevertheless, the variational approach described above is valid since all the gradients involved are given by well-defined integrals at the boundary. Moreover, all the singularities are actually contained in the function θ which is subtracted from the solution [see (4.1)-(4.3)].

5. The "interior" shaping problem

As announced in the introduction, our numerical approach is general and carries over to a large class of problems. To illustrate this, we give below numerical results for a model of the so-called "interior" shaping of liquid metals where the inductors are placed inside the liquid and the liquid confined in a bounded area: this could correspond to the shaping of a hollow tube (see the contributions by M. Crouzeix and J. Descloux in this volume). The variational problem is the same except that Ω is bounded and $m(\Omega)$ prescribed so that the only change is in the sign in front of the first term in the approximate gradient DE_{μ}^k (3.11) due to the change of sign in the normal derivative.

6. The results

The figures 1-8 which are presented next are examples of shapes which have been computed using the algorithm described in previous sections. In each case the surface tension σ and the surface S_0 of the liquid are given in addition to the distribution of current j_0 which is of the form

$$j_0 = \left(\sum_{p=1}^m \alpha_p \delta_{x_p} \right) I$$

where I is a given intensity of current, $(\delta_{x_p})_{p=1, \dots, m}$ the Dirac masses at the points $(x_p)_{p=1, \dots, m}$ in the plane and α_p adimensional coefficients which are directly indicated on the figures. Computations are made with the normalized energy

$$\int_{\Omega} |\nabla \hat{\phi}|^2 + AP(\Omega),$$

where

$$A = 2\sigma/\mu_0 I^2, \quad \hat{\phi} = \phi/\mu_0 I.$$

Tables I and II indicate for each figure the values of A , the surface S_0 and

m = number of masses,

n = number of points used to represent Ω ,

iter = the number of iterations in the algorithm.

In each case, the starting curve is a circle with surface S_0 .

TABLE I. — "Exterior" shaping problems.

| Figure n° | A | So | m | n | iter |
|-----------|-------|--------|----|-----|------|
| 1 | 0.007 | 3.1415 | 4 | 128 | 277 |
| 2 | 1. | 2. | 6 | 64 | 171 |
| 3 | 1. | 4. | 12 | 128 | 179 |
| 4 | 0.01 | 4. | 12 | 128 | 249 |

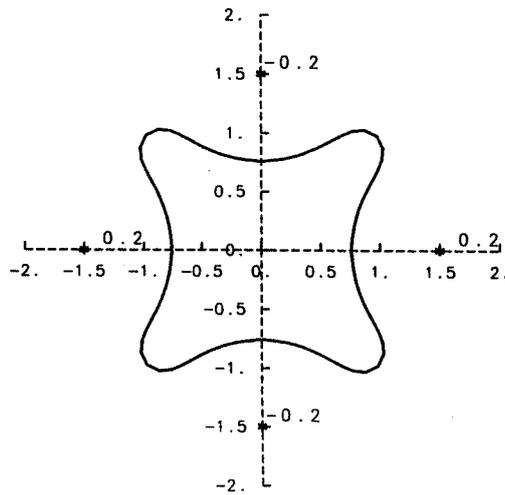


Fig. 1. — Four Dirac masses.

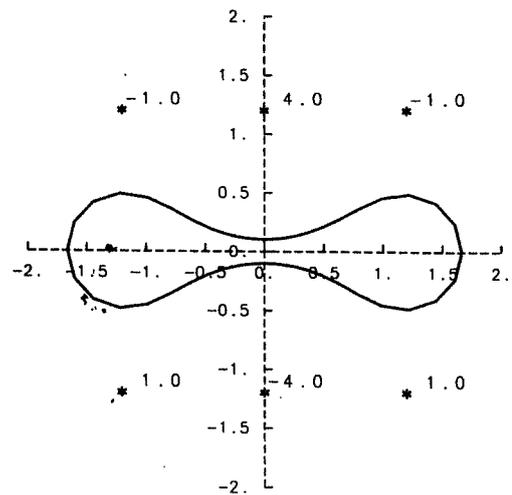


Fig. 2. — Six Dirac masses.

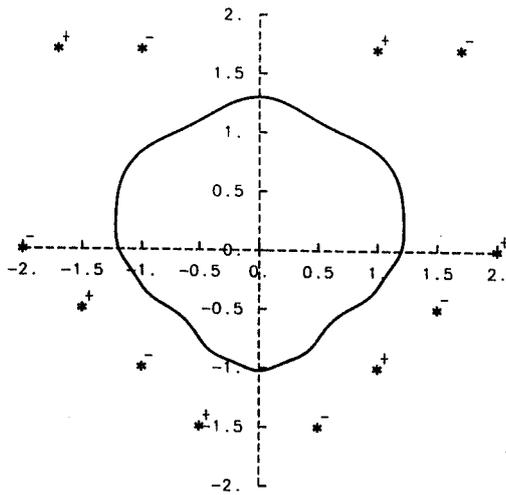
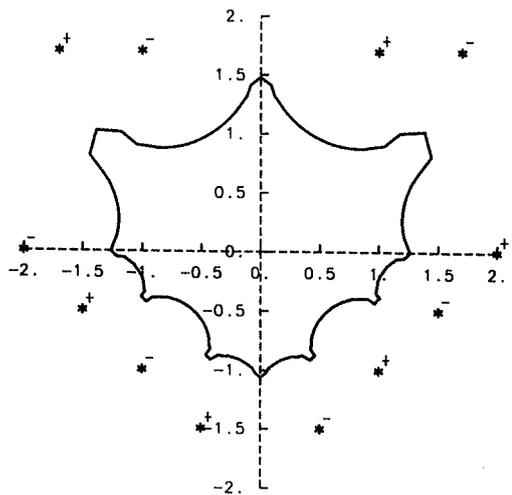
Fig. 3. — Twelve Dirac masses, $A=1$.Fig. 4. — Twelve Dirac masses, $A=0.01$.

TABLE II. — "Interior" shaping problems.

| Figure n° | A | So | m | n | iter |
|-----------|-------|----|---|-----|------|
| 5 | 1. | 1. | 2 | 128 | 122 |
| 6 | 0.001 | 1. | 4 | 64 | 46 |
| 7 | 0.01 | 1. | 4 | 64 | 70 |
| 8 | 0.01 | 1. | 4 | 64 | 76 |

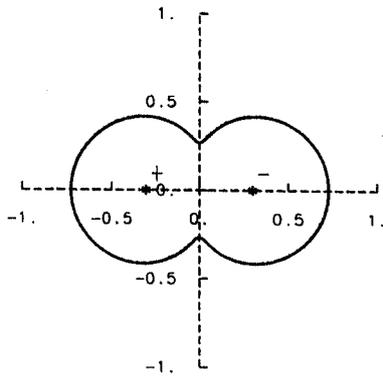


Fig. 5. — Two interior Dirac masses.

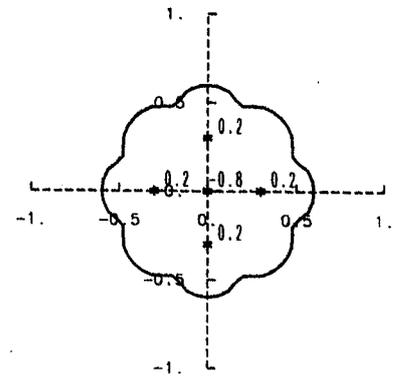


Fig. 6. — Five interior Dirac masses.

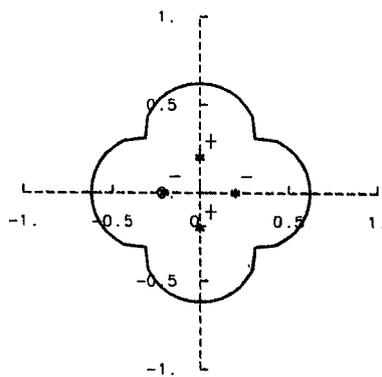
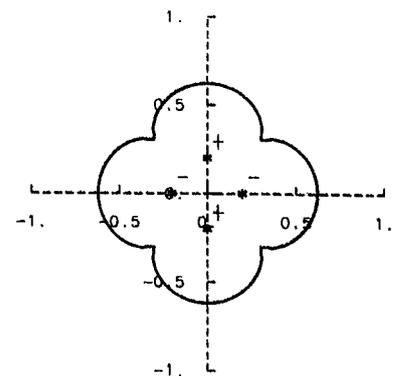
Fig. 7. — Four interior Dirac masses, $n=64$.Fig. 8. — Four interior Dirac masses, $n=128$.

Table I and Figures 1-4 are "exterior" shaping examples. The first one is classical and enables a comparison of our results with those obtained by different methods ([S, 1981]; [C & H, 1990]). The 171 iterations necessary in example 2 requires 9 seconds on a SUN 4/60. Examples 3 and 4 correspond to the same distribution of mass with $\alpha_p = \pm 1$ but with σ 100 times smaller in example 4. This explains the irregularity of the curve. Note that the curves have not been smoothed out. They are the actual piecewise linear curves obtained in the computation.

Table II and Figures 5-8 are "interior shaping" examples. Computations are faster in that case and very small surface tension can be handled. The last two examples are the same apart from a difference in the number n of nodes used in the representation of Ω .

The stability of equilibrium is under study. Some negative results in that direction can be found in [D, 1990] in the case of zero surface tension. Obviously, our optimization algorithms require at least a "numerical" stability. However, since it is based on a quasi-Newton method, it could reach stationary points which are not local minima and therefore not stable in an "energetical" sense. Note that the "interior" shaping problem leads to faster and more "stable" algorithms: this is consistent with the analysis in [D, 1990].

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