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MATHEMATICAL MODELLING AND NUMERICAL ANALYSIS
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SUPERHEATING IN A SEMI-INFINITE FILM IN THE WEAK κ LIMIT : NUMERICAL RESULTS AND APPROXIMATE MODELS (*)

by Catherine BOLLEY [1] and Bernard HELFFER [2]

Abstract — *The aim of this paper is to analyze numerically the different results concerning the superheating field for the Ginzburg-Landau equations published by the physicists In the case when the size of the film is large in comparison with the inverse of the characteristic constant κ of the material, we present an approximate model and analyze how it fits with previous numerical results and with our new computations A rigorous but partial study in the weak κ limit is presented in our other paper [8]*

Résumé — *Le but de cet article est d'analyser par des méthodes numériques les différents résultats publiés par les physiciens sur le champ de surchauffe dans les équations de Ginzburg-Landau Lorsque la largeur du film est grande par rapport à la constante κ caractéristique du matériau, nous présentons un modèle approché et le comparons aux résultats numériques précédents ainsi qu'à nos propres calculs Une étude rigoureuse, mais partielle, est présentée dans notre autre article [8] lorsque κ tend vers 0*

1. INTRODUCTION

Let us consider a superconducting film V which is submitted to an exterior magnetic field $\vec{H}_e$. According to some parameters as the thickness of the film, the intensity or the direction of the magnetic field $\vec{H}_e$ or a characteristic κ of the material, the sample can be in different states, in particular in the normal state or in the superconducting state. The phase transition phenomena are described by the Ginzburg-Landau theory which introduces a functional ϵ depending in particular on a complex wave function Ψ and on the inner magnetic potentiel A. The minima or local minima of ϵ characterize the different possible stable or metastable states. When the sample is a film and the exterior magnetic field is parallel to the surface, a modelization of

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Ginzburg-Landau [22] reduces the problem to a one dimensional problem where the wave function is real (and denoted f) and where the functional is the following :

$$\epsilon_d(f, A ; h) = \int_{-d/2}^{d/2} \left[\frac{1}{2}(1-f^2)^2 - \frac{1}{2} + \kappa^{-2} f'^2 + f^2 A^2 + (A' - h)^2\right] dx , \quad (1.1)$$

with $(f, A) \in \mathscr{H}_d = H^1(\,]-d/2, d/2[\,; \mathbb{R})^2$. Here d is proportional to the thickness of the film, h is proportional to the exterior magnetic field and κ is the Ginzburg-Landau parameter.

For a given positive h, the pairs (f, A) characterizing the different states of the superconducting films are the local and global minima of the functional ϵ_d. In particular these minima when they exist (and this is indeed the case when d is finite) are solutions in $]-d/2, d/2[$ of the following so called Ginzburg-Landau equations :

$$-\kappa^{-2} f'' + (-1 + f^2 + A^2) f = 0 \quad \text{in} \quad]-d/2, d/2[\qquad (1.2)$$

$$-A'' + f^2 A = 0 \quad \text{in} \quad]-d/2, d/2[\qquad (1.3)$$

where f and $A \in H^2(\,]-d/2, d/2[\,; \mathbb{R})$ satisfy the boundary conditions :

$$f'(\pm d/2) = 0 \quad \text{and} \quad A'(\pm d/2) = h . \qquad (1.4)$$

We get immediately the « normal solutions » $(f, A) = (0, hx + e)$ with $e \in \mathbb{R}$, which are associated to the normal state. A solution (f, A) such that f is not identically 0 will be called a superconducting solution ; it will be associated to a stable (resp. metastable) superconducting state if it is a minimum (resp. local minimum) of ϵ_d.

The main purpose of this paper is the study of a critical field which is called the superheating field. In order to give a definition, we first consider the set $\mathscr{H}_{sh}(d, \kappa)$ of the positive h's such that there exist superconducting solutions. We set :

DEFINITION 1.1 : *The superheating field $h_{sh}(d, \kappa)$ is defined as the supremum of $\mathscr{H}_{sh}(d, \kappa)$.*

In this paper we essentially analyze the asymptotic problem of the superheating field as κ tends to 0 when d is large in comparaison with $1/\kappa$. This leads us to consider a slightly different modelization which was first introduced by Ginzburg in [20] and usually called the superconducting half-space. This modelization restricts the problem to the research of symmetric solutions (f even and A odd) and considers a new normalization of the functional where

ϵ_d is replaced by $\left(\epsilon_d - \left(h^2 - \frac{1}{2}\right) d\right)$. We then restrict the problem to the interval $]-d/2, 0[$, and translate it to $]0, d/2[$. We get formally, by taking the limit $d = \infty$, the second functional:

$$\epsilon_\infty(f, A ; h) = \int_0^{+\infty} \left[\frac{1}{2}(1 - f^2)^2 + \kappa^{-2} f'^2 + f^2 A^2 + A'^2\right] dx + 2\, hA(0)\,,$$

defined for

$$(f, A) \in \mathscr{H}_\infty = \left\{(f, A) \mid (1 - f) \in H^1(\,]0,\infty[\,), A \in H^1(\,]0,\infty[\,)\right\}. \tag{1.5}$$

We remark that this choice of the functional space eliminates the normal solutions because $f \equiv 0$ does not satisfy $(1 - f) \in H^1(\,]0,\infty[\,)$.

The local extrema of the functional (if they exist) are solutions of the corresponding Ginzburg-Landau equations :

$$-\kappa^{-2} f'' - f + f^3 + A^2 f = 0 \text{ in }]0,\infty[\tag{1.6}$$

$$f'(0) = 0\,, \quad \lim_{x \to +\infty} f(x) = 1 \tag{1.7}$$

$$-A'' + f^2 A = 0 \text{ in }]0, +\infty[\tag{1.8}$$

$$A'(0) = h\,, \tag{1.9}$$

with

$$A \in H^2(\,]0, +\infty[\,), (1 - f) \in H^2(\,]0, +\infty[\,)\,.$$

Some of the boundary conditions were already introduced in the definition of our variational space but we prefer to write these conditions explicitely. We can immediately transpose the preceding definition of the superheating field to the superconducting half-space.

It is a standard result that every solution f of (1.6)-(1.9), like is a solution f of (1.2)-(1.4), satisfies $|f| \leqslant 1$ on the interval where it is defined.

We study in Section 2 the superheating field for an approximate problem which results from an improvement of an idea of P. G. de Gennes [19] and of the Orsay group [26]. We get by a rigorous proof the existence of a finite superheating field for this new problem when κ tends to 0, and give the following asymptotic formulas for $h_{sh}^{app}(\kappa)$ and for the corresponding initial condition $f_{0\,sh}^{app} = f(0)$:

$$h_{sh}^{app} = \kappa^{-1/2}\, 2^{-3/4} (1 + 5.2^{-7/2}\, \kappa \ln(\kappa^{-1}) + \mathcal{O}(\kappa)) , \tag{1.10}$$

$$f_{0\,sh}^{app} = \frac{1}{\sqrt{2}} \left(1 - \frac{1}{8\sqrt{2}} \kappa \ln(\kappa^{-1}) + \mathcal{O}(\kappa) \right) . \tag{1.11}$$

We get by this study an approximate value for the superheating field, but we have no control of the error between the approximate model and the initial problem. These results have been announced in [3].

Section 3 gives some qualitative properties of the solutions of a family of initial value problems associated to the system (1.6)-(1.9) and classify the solutions according to their asymptotic behavior. These problems will be used in the numerical treatment of the last section.

Section 4 first analyzes the different results, formulas or numerical computations, concerning the superheating field appearing in the physical literature and compare them to our own formula obtained in Section 2. The divergence of a part of these results, essentially for small values of κ, leads us to a more careful numerical analysis of the problem in the half space. This is the object of the second part of Section 4 where we use shooting methods on the initial value problem associated to Problem (1.6)-(1.9) and a semi-implicite Runge-Kutta method in order to compute solutions of the Ginzburg-Landau equations. We detail the numerical tests that we have used, but a theoretical justification is missing.

Our numerical results agree of course for κ small with the formula of P. G. de Gennes and the Orsay Group ([19] and [26]) :

$$\lim_{\kappa \to 0} h_{sh}(\kappa)\, \kappa^{1/2} = 2^{-3/4} , \tag{1.12}$$

but suggest an expansion for κh^2 in power of κ and not in $\kappa \ln(\kappa)$ as given in (1.10). Actually they fit relatively well with the asymptotic formula given by H. Parr in [27].

Rigorous results concerning this formula will be given in [8] and [10] but the study of the approximate model has been important in the research of the subsolutions constructed in [8] for the exact model.

In a previous version [9], we have also studied in the same spirit as in Section 2 the case of a bounded interval $[-d/2, d/2]$ when d large in comparison with $1/\kappa$. This part is not reproduced here.

Acknowledgements : These results have been announced in [6], [7], [3], at the working seminar in E.N.S. and at the Congrès National d'Analyse Numérique in Karellis. We would like to thank all the organizers of these seminars or conferences and also A. Bonnet for useful suggestions.

We thank also M. Crouzeix for his constructive remarks leading to improvements of the previous version [9], in the presentation of the approximate model.

2. STUDY OF AN APPROXIMATE MODEL, WITH κ SMALL

In order to study the superheating field when the size of the interval is large in comparison with $1/\kappa$, we consider the problem in a semi-infinite interval which plays the role of a simplified model.

Using a method of successive approximations, Ginzburg [21] has found that for very small κ, the superheating field satisfies :

$$h_{sh} \approx 0{,}89\, \kappa^{-1/2} H_c ,$$

where H_c is the critical thermodynamic field of the bulk material ($H_c = 2^{-1/2}$). Then, from a non rigorous discussion on approximate solutions for the GL equations (1.6)-(1.9), the Orsay group [26] and P. G. de Gennes [19] deduced in 1966 the following estimate for this critical field :

$$h_{sh} = 2^{-1/4} \kappa^{-1/2} H_c \approx 0{,}8409\, \kappa^{-1/2} H_c . \tag{2.1}$$

We will go back to this problem by analyzing carefully a more explicit approximate problem. No rigorous proof exists measuring the error between this approximate model and the initial problem, but we shall compare in a next section the numerical results given in the literature and the results given by this model. This model will appear to be good far from the superheating field (which is not the case of the P. G. de Gennes's formula).

We keep the idea of P. G. de Gennes [19] and the Orsay group [26] who split the GL equations in two simpler boundary value problems : one problem on some interval $]0, D[$ where f is supposed to be constant (this fact means that for small κ the function f is nearly constant (see [21] and [5] Section 4), and a problem on $]D, +\infty[$ where A is chosen equal to 0 (this means that the Meissner effect is satisfied). This leads us to restrict the initial variational space $\mathscr{H}_\infty$ of the GL-functional to a smaller subset.

Let us first introduce the space $U_\infty(f_0, D)$, defined for $(f_0, D) \in\ ]-1, 1] \times [0, +\infty[$ by :

$$U_\infty(f_0, D) = \{(f, A) \in \mathscr{H}_\infty ; f = f_0 \text{ on }]0, D[, A = 0 \text{ on }]D, +\infty[\} ,$$

and let us consider the problem of minimization for the GL functional over $U_\infty(f_0, D)$.

PROPOSITION 2.1 : *Let* $(f_0, D, h) \in]-1, 1] \times [0,\infty[\times [0,\infty[$. *Then the restriction to* $U_\infty(f_0, D)$ *of the functional* $(f, A) \to \epsilon_\infty(f, A ; h)$ *admits an unique critical point in* $U_\infty(f_0, D)$. *This point is a minimum for* ϵ_∞ *over* $U_\infty(f_0, D)$ *and*

$$\epsilon_0(f_0, D ; h) \equiv \inf_{(f, A) \in U_\infty(f_0, D)} \epsilon_\infty(f, A ; h) , \tag{2.2}$$

is given by

$$\epsilon_0(f_0, D ; h) = \frac{D}{2}\left[(1 - f_0^2)^2 - 2h^2 \frac{\tanh Df_0}{Df_0}\right] + \frac{\sqrt{2}}{3\kappa}(1 - f_0)^2 (f_0 + 2) . \tag{2.3}$$

Proof :
For every $(f, A) \in U_\infty(f_0, D)$

$$\epsilon_\infty(f, A ; h) = \frac{D}{2}(1 - f_0^2)^2 + e_1(A) + e_2(f) ,$$

where

$$e_1(A) = \int_0^D (f_0^2 A^2 + A'^2)\, dx + 2\, hA(0) ,$$

$$e_2(f) = \int_D^{+\infty} \left(\frac{1}{2}(1 - f^2)^2 + \kappa^{-2} f'^2\right) dx .$$

The functional $A \to e_1(A)$ is strictly convex on the domain $U_1 = \{A \in H^1(]0, D[) ; A(D) = 0\}$; its minimum is reached for A such that $-A'' + f_0^2 A = 0$ in $]0, D[$ with $A'(0) = h$ and $A(D) = 0$. We then get :

$$A(x) = -\frac{h}{f_0 \cosh(f_0 D)} \sinh(f_0(D - x)) \quad \text{for} \quad x \in [0, D] . \tag{2.4}$$

The infimum over U_1 of e_1 is then equal to :

$$\inf_{A \in U_1} e_1(A) = -\frac{h^2}{f_0} \tanh(f_0 D) \quad \text{when} \quad f_0 \neq 0 ,$$

$$\inf_{A \in U_1} e_1(A) = -h^2 D \quad \text{when} \quad f_0 = 0 .$$

The functional $f \to e_2(f)$ is defined on $U_2 = \{f \,;\, (1-f) \in H^1(\,]D, +\infty[\,),\ f(D) = f_0\}$. Its critical points satisfy

$$-\kappa^{-2} f'' - f + f^3 = 0 \text{ on }]D, +\infty[\ , \tag{2.5}$$

$$f(D) = f_0\,,\ (1-f) \in H^1(\,]D, \infty[\,)\,.$$

Let us prove the existence and uniqueness of a solution for (2.5).

Multiplying the equation by f' and integrating gives the conservation of energy :

$$\kappa^{-2} f'(x)^2 + f(x)^2 - \tfrac{1}{2} f(x)^4 = \text{Const.}\,,$$

where the constant is computed, using the boundary condition at $+\infty$, as equal to $\frac{1}{2}$. We get

$$f'(x) = \pm \frac{\kappa}{\sqrt{2}} (1 - f(x)^2)\,.$$

The function f' is positive for large x because $|f| \leq 1$ and f tends to 1 as $x \to +\infty$. The only points where f' can vanish are points such that $f(x) = \pm 1$, but if such points exist $f \equiv \pm 1$ on $]D, \infty[$. Therefore, the condition $f(D) = f_0$ implies that $f' > 0$ on $]D, +\infty[$ unless when $f_0 = 1$. In any case, we have consequently

$$f'(x) = + \frac{\kappa}{\sqrt{2}} (1 - f(x)^2)\,. \tag{2.6}$$

We get by a new integration, when $f_0 \in\ ]-1, 1[$

$$f(x) = \tanh\left(\frac{\kappa}{\sqrt{2}} (x - x_0)\right) \quad \text{for } x \in [D, +\infty[\ , \tag{2.7}$$

with

$$x_0 = D - \frac{\sqrt{2}}{\kappa} \tanh^{-1}(f_0)\,. \tag{2.8}$$

When $f_0 = 1$, then $f \equiv 1$.

Therefore, for $f_0 \in\ ]-1, +1]$:

$$\inf_{f \in U_2} e_2(f) = \kappa^{-1} \int_D^{\infty} \sqrt{2} (1 - f(x)^2) f'(x)\, dx = \frac{\sqrt{2}}{3\kappa} (1 - f_0)^2 (f_0 + 2)\,.$$

The relations (2.4) and (2.7)-(2.8) determine a unique element in $U_\infty(f_0, D)$. We get Proposition 2.1.

The research of a pair $(f, A) \in \mathscr{H}_\infty$ such that $\epsilon_\infty(f, A\,;h)$ is locally minimal, is then replaced, for the approximate problem, by the research of $D \geqslant 0$ and $f_0 \in \,]-1, 1]$ s.t. $\epsilon_0(f_0, D\,;h)$ is locally minimal ([3]).

Remark 2.2 : For $0 < f_0 < 1$, we have

$$\epsilon_0(-f_0, D\,;h) = \epsilon_0(f_0, D\,;h) + 2(3 - f_0^2) f_0 \geqslant \epsilon_0(f_0, D\,;h)\,. \qquad (2.9)$$

Therefore, when we restrict the study to the f_0's such that $f_0 \in [0, 1]$, we perhaps eliminate local minima but no global minima.

In order to show, in the case when $0 < h < \frac{1}{\sqrt{2}}$, the existence of a minimum, we shall prove the following proposition :

PROPOSITION 2.3 : *For $0 < h < \frac{1}{\sqrt{2}}$, the functional ϵ_0 is semibounded on the set $\mathscr{V}$ of the pairs (f_0, D) s.t. $f_0 \in \,]-1, 1[$ and $D \geqslant 0$, and the minimum is reached for a pair (f_0, D) such that*

$$f_0 \geqslant \max\left\{\sqrt{1 - \sqrt{2}\,h}\,;\bar{f}_0\right\}, \qquad (2.10)$$

where $\bar{f}_0 \approx 0.78$ is the solution in $]0, 1[$ of the equation

$$f_0^{\frac{10}{3}} - 2 f_0^{\frac{4}{3}} + 1 = 0\,.$$

Proof :

We first prove the semiboundedness.

The relation (2.9) reduces the study to pairs (f_0, D) such that $f_0 \geqslant 0$.

Now, we have from (2.3) the following lower bound for $\epsilon_0(f_0, D\,;h)$:

$$\epsilon_0(f_0, D\,;h) \geqslant \frac{D}{2}\left[(1 - f_0^2)^2 - 2h^2\right] + \frac{\sqrt{2}}{3\kappa}(2 - 3f_0 + f_0^3)\,.$$

Now, for $h < \frac{1}{\sqrt{2}}$, we can find $\rho > 0$, $\rho \leqslant 1$ such that $(1 - \rho^2)^2 - 2h^2 > 0$ and then :

$$\forall f_0 \in [0, \rho] \text{ and } D \geqslant 0 : \epsilon_0(f_0, D\,;h) \geqslant \frac{\sqrt{2}}{3\kappa}(2 - 3\rho)\,. \qquad (2.11)$$

([3]) Another approach was used in an earlier version distributed as a preprint of ECN [9] We follow here a suggestion of M Crouzeix

For $f_0 \in [\rho, 1]$, coming back to (2.3), we write

$$\epsilon_0(f_0, D ; h) \geqslant -\frac{h^2}{f_0} + \frac{\sqrt{2}}{3\kappa}(2 - 3f_0 + f_0^3), \tag{2.12}$$

which gives

$$\epsilon_0(f_0, D ; h) \geqslant -\frac{h^2}{\rho} + \frac{\sqrt{2}}{3\kappa}(-1 + \rho^3), \tag{2.13}$$

and the first part of the proposition.

Let us improve this result.

Proof of (2.10) : Let

$$\alpha_0(f_0, h) = \inf_{D \geqslant 0} \epsilon_0(f_0, D ; h). \tag{2.14}$$

If $1 - f_0^2 \geqslant \sqrt{2}\, h$, the minimum for ϵ_0 with respect to D is reached for $D = 0$. Then

$$\alpha_0(f_0, h) = \frac{\sqrt{2}}{3\kappa}(1 - f_0)^2(f_0 + 2) \geqslant 0.$$

When $1 - f_0^2 < \sqrt{2}\, h$, we get $|f_0| > \sqrt{1 - \sqrt{2}\, h}$, then $f_0 \neq 0$. A critical value for ϵ_0 with respect to D is given by the vanishing of $\frac{\partial \epsilon_0}{\partial D}(f_0, D ; h)$. This gives

$$\tanh(Df_0) = \frac{f_0}{|f_0|}\left(1 - \frac{(1 - f_0^2)^2}{2h^2}\right)^{1/2}.$$

Now, for every $D \geqslant 0$:

$$\frac{\partial^2 \epsilon_0}{\partial D^2}(f_0, D ; h) = 2h^2 f_0 \cdot \left(1 - \tanh^2(f_0 D)\right) \cdot \tanh(f_0 D),$$

which implies that D_0 given by

$$\tanh(D_0 |f_0|) = \sqrt{1 - \frac{(1 - f_0^2)^2}{2h^2}} \tag{2.15}$$

leads to a minimum for $D \to \epsilon_0(f_0, D ; h)$. We get for $|f_0| > \sqrt{1 - \sqrt{2}\, h}$:

$$\alpha_0(f_0, h) = \frac{D_0}{2}(1 - f_0^2)^2 - \frac{h^2}{f_0}\tanh(D_0 f_0) + \frac{\sqrt{2}}{3\kappa}(1 - f_0)^2(f_0 + 2),$$

with D_0 given by (2 15)

We have in particular when $f_0 = 1 - \epsilon$

$$\alpha_0(1 - \epsilon, h) = -h^2 (1 + \epsilon) + \mathcal{O}_h(\epsilon^2 |\ln \epsilon|) \qquad (2\ 16)$$

This shows that the minimum of $f_0 \to \alpha_0(f_0, h)$ is strictly lower than $-h^2$, and consequently reached for an $f_0 = \hat{f}_0$ such that $\hat{f}_0^2 > 1 - \sqrt{2}\, h$ and $f_0 > 0$ At this minimum, using that $\tanh x \leqslant x$, we have

$$0 \geqslant \alpha_0(\hat{f}_0, h) + h^2 \geqslant \frac{\tanh(D_0 \hat{f}_0)}{2\hat{f}_0}(1 - \hat{f}_0^2)^2 - \frac{h^2 \tanh(D_0 \hat{f}_0)}{\hat{f}_0} + h^2$$

$$= \frac{h^2}{\hat{f}_0}\left[\hat{f}_0 - \left(1 - \frac{(1 - \hat{f}_0^2)^2}{2h^2}\right)^{\frac{3}{2}}\right]$$

We get

$$\hat{f}_0^{\frac{2}{3}} < 1 - \frac{(1 - \hat{f}_0^2)^2}{2h^2} \Leftrightarrow \frac{(1 - \hat{f}_0^2)^2}{1 - \hat{f}_0^{\frac{2}{3}}} < 2h^2 \leqslant 1$$

Therefore we have the inequality

$$\hat{f}_0^{2/3} - 2\hat{f}_0^2 + \hat{f}_0^4 < 0$$

By studying the variation of $f_0 \to f_0^{10/3} - 2f_0^{4/3} + 1$, we observe that it has a unique zero $\tilde{f}_0$ in $]0, 1[$ and we consequently get

$$\hat{f}_0 > \tilde{f}_0 ,$$

with $\quad 0\ 78 < \tilde{f}_0 < 0\ 79$

We shall show in [8] that the GL functional ϵ_∞ is also semibounded in $\mathcal{H}_\infty$ for $h < \frac{1}{\sqrt{2}}$ See also Remark 7 3 in [8]

We are now interested in the case when $h > \frac{1}{\sqrt{2}}$ We have in that case

PROPOSITION 2 4 *For $h > \frac{1}{\sqrt{2}}$, the functional ϵ_0 is not semibounded on the set $\mathcal{V}$*

Proof For every $f_0 \in [0, 1]$, using the inequality $\tanh(x) \geq x - \frac{x^3}{3}$ for $x \geq 0$, we have

$$\epsilon_0(f_0, D, h) \leq \frac{D}{2}\left(1 - 2h^2 + \frac{2}{3}(f_0 D)^2 h^2\right)$$

$$- \frac{Df_0^2}{2}(2 - f_0^2) + \frac{\sqrt{2}}{\kappa}(2 - 3f_0 + f_0^3), \quad (2\ 17)$$

But for any $h > \frac{1}{\sqrt{2}}$, there exists a constant a such that $\left(1 - 2h^2 + \frac{2}{3}a^2 h^2\right) < 0$ Consequently, if $(f_0^{(n)})$ is a sequence tending to 0 when n tends to $+\infty$, and if $D_n = a / f_0^{(n)}$, then $\epsilon_0(f_0^{(n)}, D_n, h)$ tends to $-\infty$ as the first term when n tends to $+\infty$ This shows that ϵ_0 is not semibounded

Proposition 2 4 has an important consequence for the GL functional ϵ_∞ The functional ϵ_0 has actually been introduced by restriction of the GL functional ϵ_∞ to a smaller set Therefore, it results immediately from Proposition 2 4 the following corollary

COROLLARY 2 5 *If $h > \frac{1}{\sqrt{2}}$, the GL functional ϵ_∞ is not semibounded*

However, as an immediate consequence of (2 13), we have the following result for ϵ_0

PROPOSITION 2 6 *For every $h > 0$ and every $\rho > 0$, the functional ϵ_0 is semibounded on the subset $\mathcal{V}_\rho$ of the (f_0, D) s t $f_0 \geq \rho$ and $D \geq 0$*

A consequence of Proposition 2 4 is the non existence of any global minimum for the two functionals for $h > \frac{1}{\sqrt{2}}$, and we can only hope for local minima for ϵ_0

Remark 2 7 (4) For $\frac{1}{\sqrt{2}} < h \leq \sqrt{1 - \left(\frac{7}{16}\right)^{\frac{3}{2}} + \frac{5\sqrt{2}}{24\kappa}}$, the function $f_0 \to \alpha_0(f_0, h)$ defined as in (2 14) admits a local minimum which is reached by an $f_0 = f_0^{\min} \in \left]\frac{1}{2}, 1\right[$

Indeed, using once again that $\tanh x \leq x$ for $x \geq 0$

$$\epsilon_0\left(\frac{1}{2}, D, h\right) + h^2 = \epsilon_0\left(\frac{1}{2}, D, \frac{1}{\sqrt{2}}\right) + \frac{1}{2} + \left(h^2 - \frac{1}{2}\right)\left(1 - 2\tanh\frac{D}{2}\right)$$

$$\geq \alpha_0\left(\frac{1}{2}, \frac{1}{\sqrt{2}}\right) + \frac{1}{2} - \left(h^2 - \frac{1}{2}\right)$$

$$\geq 1 - \left(\frac{7}{16}\right)^{3/2} + \frac{5\sqrt{2}}{24\kappa} - h^2$$

(4) This remark was suggested to us by M Crouzeix

This gives the result, using (2.16). We note that $1-\left(\frac{7}{16}\right)^{\frac{3}{2}} \sim 0.71$.

Moreover, because

$$\lim_{f_0 \to 0} \alpha_0(f_0, h) = -\infty \tag{2.18}$$

when $h > \frac{1}{\sqrt{2}}$, we get the existence of a local maximum for $f_0 \to \alpha_0(f_0, h)$ in $]0, f_0^{\min}[$.

We shall now show the following result :

PROPOSITION 2.8 : *Let $\mathcal{H}_{sh}^{(0)}(\kappa)$ be the set of the $h > 0$ such that there exists a local minimum for the functional ϵ_0. Then, there exists $\kappa_0 > 0$ such that, for $0 < \kappa \leq \kappa_0$, the set $\mathcal{H}_{sh}^{(0)}(\kappa)$ is an interval $(0, h_{sh}^{app}]$ where h_{sh}^{app} and the corresponding f_0, denoted by $f_{0\,sh}^{app}$, satisfy :*

$$h_{sh}^{app} = \kappa^{-1/2} 2^{-3/4} \left(1 - 5.2^{-7/2} \kappa \ln(\kappa) + \mathcal{O}(\kappa)\right), \tag{2.19}$$

$$f_{0,sh}^{app} = 2^{-1/2} \left(1 + 2^{-7/2} \kappa \ln \kappa + \mathcal{O}(\kappa)\right). \tag{2.20}$$

Proof :

Step 1 : The Euler equations

The critical points of the functional are given by the vanishing of the derivatives $\partial\epsilon_0/\partial f_0$ and $\partial\epsilon_0/\partial D$. Let us write $\partial\epsilon_0/\partial f_0$:

$$\left(\frac{\partial \epsilon_0}{\partial f_0}\right)(f_0, D; h) = \frac{h^2}{f_0^2} \tanh(f_0 D) - \frac{h^2 D}{f_0}\left(1 - \tanh^2(f_0 D)\right) - 2 D f_0 (1 - f_0^2) - \frac{\sqrt{2}}{\kappa}(1 - f_0^2). \tag{2.21}$$

As for the constant model considered in [5], the condition $\partial\epsilon_0/\partial f_0 = 0$ gives

$$h^2 = \frac{f_0^2 (1 - f_0^2)\left(\frac{\sqrt{2}}{\kappa} + 2 D f_0\right)}{\tanh(f_0 D) - D f_0 \left(1 - \tanh^2(f_0 D)\right)}. \tag{2.22}$$

On the other hand

$$\left(\frac{\partial \epsilon_0}{\partial D}\right)(f_0, D; h) = -h^2\left(1 - \tanh^2(f_0 D)\right) + 2^{-1}(1 - f_0^2)^2 ; \tag{2.23}$$

so that the equation $\partial \epsilon_0 / \partial D = 0$ gives the following relation :

$$h^2 = \frac{1}{2} (1 - f_0^2)^2 \cosh^2 (f_0 D) . \tag{2.24}$$

Remark 2.9 : The relation (2.24) can also be understood as a consequence of the conservation law for the GL system. We recall that the GL system can be rewritten as an hamiltonian system which admits the following conservation law, for any $x \in [0, +\infty[$,

$$\kappa^{-2} f'^2(x) + A'^2(x) - \frac{1}{2} (1 - f^2(x))^2 - A^2(x) f^2(x) = \text{Const.} , \tag{2.25}$$

where the constant is proved to be 0 by taking the limit $x \to +\infty$.

We get, in particular, when $x = 0$

$$h^2 = \frac{1}{2} (1 - f(0)^2)^2 + f(0)^2 A(0)^2 . \tag{2.26}$$

At the critical value for ϵ_∞ the function A satisfies $A(0) = -\dfrac{h \tanh (f_0 D)}{f_0}$ and then (2.26) allows us to find again (2.24).

Remark 2.10 : This conservation law was used in the argument of the Orsay group but appears unclear in the details.

Neglecting $2 D f_0$ in (2.22) in comparison with $\sqrt{2} \kappa^{-1}$ and using the approximation $\tanh (f_0 D) \approx 1$, we get as an approximation of this equation the following formula

$$h^2 \approx f_0^2 (1 - f_0^2) \sqrt{2} \kappa^{-1}$$

which is the formula given in [19], but these approximations are only justified for $f_0 D$ large. Our derivation seems more natural.

Step 2 : The asymptotic behavior for h as fonction of f_0 and D

The elimination of h between (2.22) and (2.24) gives us a relation between D and f_0 :

$$\frac{1}{2} (1 - f_0^2) \cosh^2 (f_0 D) = \frac{f_0^2 \left(\sqrt{2} \kappa^{-1} + 2 D f_0 \right)}{\tanh (f_0 D) - D f_0 \left(1 - \tanh^2 (f_0 D) \right)} \tag{2.27}$$

Let us introduce new parameters

$$u = f_0^2 \quad \text{and} \quad y = D f_0 .$$

We can then rewrite (2.27) as

$$u(2^{3/2}\kappa^{-1} + 4y) - (1-u)(\sinh y \cosh y - y) = 0 . \tag{2.28}$$

Then

$$u = \frac{\sinh y \cosh y - y}{\sinh y \cosh y + (3y + 2^{3/2}\kappa^{-1})} \tag{2.29}$$

or

$$1 - u(y) = \frac{4y + 2^{3/2}\kappa^{-1}}{\frac{1}{2}\sinh(2y) + (3y + 2^{3/2}\kappa^{-1})} . \tag{2.30}$$

We can then rewrite h as function of y:

$$h = \frac{1}{\sqrt{2}}(1-u)\cosh y , \tag{2.31}$$

with $u = u(y)$ given by (2.30). We then get:

$$h(y) = \frac{\sqrt{2}(4y+\lambda)(\exp y + \exp - y)}{12y + 4\lambda + \exp 2y - \exp - 2y} \tag{2.32}$$

where $\lambda = 2^{3/2}\kappa^{-1}$.

Let us consider $h(y)$ for y small. We get:

$$h(y) = \frac{1}{\sqrt{2}}\left(1 + \frac{y^2}{2} + \mathcal{O}(y^3)\right) . \tag{2.33}$$

Now, for large y,

$$h(y) = 4\sqrt{2}\, y \exp - y + \mathcal{O}(\exp - y) .$$

When y tends to 0, $h(y)$ tends to $1/\sqrt{2}$, and when y tends to $+\infty$, $h(y)$ tends to 0. Moreover, the function $y \rightarrow h(y)$ is an increasing function of y for $y > 0$ small and has a local minimum at $y = 0$. We deduce from these computations that there exists at least one strictly positive y such that $\partial h/\partial y = 0$ and h is maximal. Moreover, this maximum is larger than $1/\sqrt{2}$.

Following the intuition of the Orsay group [26], we calculate y and h such that this relation is satisfied ; we denote by $f(y)$ and $g(y)$ the numerator and the denominator of $y \to h(y)$ in (2.32) :

$$f(y) = \sqrt{2}(4y + \lambda)(\exp y + \exp - y)$$

$$g(y) = 12y + 4\lambda + \exp 2y - \exp - 2y .$$

We write that :

$$\partial h/\partial y = 0 \text{ if and only if } f'g = fg' ,$$

with

$$2^{-1/2} f'(y)\, g(y) =$$

$$(4\lambda + \exp 2y + 12y - \exp - 2y)$$

$$\times (\lambda \exp y + 4y \exp y - \lambda \exp - y + 4 \exp y - 4y \exp - y + 4 \exp - y)$$

$$2^{-1/2} f(y)\, g'(y) =$$

$$(\lambda \exp y + 4y \exp y + \lambda \exp - y + 4y \exp - y)$$

$$\times (2 \exp 2y + 12 + 2 \exp - 2y) .$$

The equation $f'g - fg' = 0$ can be considered as a second order equation in λ. We have :

$$2^{-1/2}(f'(y)\, g(y) - f(y)\, g'(y)) = \alpha(y)\, \lambda^2 + \beta(y)\, \lambda + \gamma(y) ,$$

with

$$\alpha(y) = 4(\exp y - \exp - y)$$

$$\beta(y) = 4(4y \exp y + 4 \exp y - 4y \exp - y + 4 \exp - y)$$

$$+ (\exp y - \exp - y)(\exp 2y + 12y - \exp - 2y)$$

$$- (\exp y + \exp - y)(2 \exp 2y + 12 + 2 \exp - 2y)$$

$$\gamma(y) = (\exp 2y + 12y - \exp - 2y)$$

$$\times (4y \exp y + 4 \exp y - 4y \exp - y + 4 \exp - y)$$

$$- 4y(\exp y + \exp - y)(2 \exp 2y + 12 + 2 \exp - 2y) .$$

We then observe that the coefficient $\alpha(y)$ of λ^2 is equal to $8\sqrt{2} \sinh y$ which is strictly positive for $y > 0$ and that the coefficient $\gamma(y)$ behaves like

$-4\sqrt{2}\, y \exp 3y$ for large y Therefore we obtain the existence for y large positive of a unique root $\lambda(y) > 0$ of the second order equation We shall now show that its asymptotic behavior is that of $\exp 2y/4$, and it will then be easy to prove that conversely for λ large positive there exists a unique positive y such that $h'(y) = 0$

In order to compute the positive root, denoted by $\lambda_+(y)$, we use that

$$\lambda_+(y) = \frac{-\beta(y) + \sqrt{\beta(y)^2 - 4\,\alpha(y)\,\gamma(y)}}{2\,\alpha(y)}$$

we then take the asymptotic for large y and, in a second step, deduce an asymptotic formula for y as a function of λ

We have

$$\alpha(y)^{-1} = 4^{-1}(\exp - y)\,(1 + \exp - 2y) + \mathcal{O}(\exp - 3y)$$

$$\beta(y) = -\exp 3y\,(1 - 28y \exp - 2y + \mathcal{O}(\exp - 2y))$$

$$\gamma(y) = -4y \exp 3y\,(1 - y^{-1} - 12y \exp - 2y + \mathcal{O}(\exp - 2y))$$

Therefore the discriminant satisfies for large y

$$\Delta(y) = \exp 6y\,(1 + 8y \exp - 2y + \mathcal{O}(\exp - 2y))$$

This gives us the following formula for $\lambda_+(y)$

$$\lambda_+(y) = 4^{-1} \cdot \exp 2y\,(1 - 12y \exp - 2y + \mathcal{O}(\exp - 2y)) \tag{2 34}$$

We get that for λ large enough there exists a unique $y = y_{sh}$ giving the maximum of $y \to h(y)$, and this y_{sh} has the following expansion for large λ

$$y_{sh} = \frac{1}{2}\ln(\lambda) + \ln(2) + \frac{3}{4}\frac{\ln(\lambda)}{\lambda} + \mathcal{O}\left(\frac{1}{\lambda}\right) \tag{2 35}$$

Now when $\frac{1}{\sqrt{2}} < h < h(y_{sh})$, there exists two values $y_{\min}(h)$ and $y_{\max}(h)$ of y such that

$$y_{\min}(h) < y_{sh} < y_{\max}(h)$$

and

$$h = h(y_{\min}(h)) = h(y_{\max}(h))$$

Using (2.31) we can compute the value of h corresponding to the critical y_{sh}. We first have from (2.35) :

$$\exp 2y_{sh} = 4\,\lambda + 6 \ln(\lambda) + \mathcal{O}(1)\,.$$

Then

$$1 - u(y_{sh}) = 2^{-1} + 2^{-2}\lambda^{-1} \ln(\lambda) + \mathcal{O}(\lambda^{-1})\,, \tag{2.36}$$

so that, using (2.31)

$$h(y_{sh}) = 2^{-3/2}\sqrt{\lambda}\,.\,(1 + 5\,.\,2^{-2}\lambda^{-1}\ln(\lambda) + \mathcal{O}(\lambda^{-1}))\,.$$

Then, since $\lambda = 2^{3/2}\kappa^{-1}$, we find

$$y_{sh} = 2^{-1}\ln(\kappa^{-1}) + 7\,.\,2^{-2}\ln 2 + \mathcal{O}(\kappa \ln(\kappa^{-1}))\,, \tag{2.37}$$

$$u(y_{sh}) = 2^{-1}(1 + 2^{-5/2}\kappa \ln \kappa + \mathcal{O}(\kappa))\,. \tag{2.38}$$

Then we get as a possible candidate for an approximate superheating field :

$$h_{sh}^{app} = h(y_{sh}) = \kappa^{-1/2}2^{-3/4}(1 - 5\,.\,2^{-7/2}\kappa\ln\kappa + \mathcal{O}(\kappa)) \tag{2.39}$$

The corresponding f_0 and D satisfy :

$$f_{0\,sh}^{app} = u^{1/2}(y_{sh}) = 2^{-1/2}(1 + 2^{-7/2}\kappa \ln(\kappa) + \mathcal{O}(\kappa))\,, \tag{2.40}$$

and

$$D_{sh} = \frac{y_{sh}}{f_{0\,sh}^{app}} = 2^{-1/2}\ln(\kappa^{-1}) + 7\,.\,2^{-3/2}\ln 2 + \mathcal{O}(\kappa\,.\,(\ln\kappa)^2)\,. \tag{2.41}$$

Remark 2.11 : We have not investigated two points. We have not verified that the constructed solution $(y_{\max}(h), u(y_{\max}(h)))$ for given h corresponds effectively to a local minimum of the functional, while the other solution $(y_{\min}(h), u(y_{\min}(h)))$ corresponds to a saddle point. See however Remark 2.7. Another crucial point will be to prove an estimate between the « approximate » superheating field and the real one. It will be very convenient to prove an estimate like :

$$|h_{sh} - h_{sh}^{app}| \leqslant C|\ln\kappa|\,.\,\sqrt{\kappa}\,.$$

But we are unable to prove for the moment the weaker :

$$h_{sh}/h_{sh}^{app} = 1 + o(1) \quad \text{as } \kappa \to 0\,.$$

We shall discuss in Section 3 numerical results on this problem and we shall see that, if the first term of the expansion (2.39) is confirmed, it is not the case for the second.

Now, using very accurate computations of subsolutions for the GL equations, we show in [8] that there exists a constant C_0 such that :

$$\kappa^{1/2} h_{sh}(\kappa) \geqslant 2^{-3/4} + C_0 \kappa + \mathcal{O}(\kappa^2) ;$$

which gives a nearly optimal lower bound of the superheating field if we compare the formulas given by P. G. de Gennes [19] and H. Parr [27], and Section 3.

About the branching point at $\left(f_0 = 0, h = \frac{1}{\sqrt{2}}\right)$.

Another interesting question concerning the solutions (f, A) of the GL equations, is the asymptotic behavior for h and $A(0)$ as f_0 tends to 0. We have

LEMMA 2.12 : *Let (f, A) be a solution of the approximate problem such that $f(0) = f_0$ and $A'(0) = h$, then, as f_0 tends to 0,*

$$(a)\ h = \frac{1}{\sqrt{2}} + \left(\frac{3}{\kappa}\right)^{2/3} 2^{-7/6} f_0^{4/3} + \mathcal{O}_\kappa(f_0^2) ,$$

$$(b)\ A(0) = -\left(\frac{3}{2\kappa}\right)^{1/3} f_0^{-\frac{1}{3}} + \mathcal{O}_\kappa(f_0^{1/3}) , \tag{2.42}$$

$$(c)\ \epsilon_0(f_0, D, h) = \frac{2\sqrt{2}}{3\kappa} + \mathcal{O}_\kappa(f_0^{1/3}) .$$

Proof : We come back to the variables $u = f_0^2$ and $y = f_0 D$. Using (2.29) and the inequality $\sinh y \cosh y - y > 0$ for $y > 0$, we get that

$$f_0 \text{ tends to } 0 \quad \text{if and only if} \quad y = f_0 D \text{ tends to } 0 .$$

The equation (2.29) gives for small f_0 :

$$u = \frac{\kappa}{3\sqrt{2}} y^3 + \mathcal{O}(y^4) ,$$

or

$$y = \left(3\sqrt{2}\,\kappa^{-1}\right)^{1/3} u^{1/3} + \mathcal{O}(u^{2/3}) ;$$

so that (a) results immediately from (2.33).

Now,

$$A(0) = -\frac{h}{u^{1/2}} \tanh(y)$$

$$= -\left(3\sqrt{2}\,\kappa^{-1}\right)^{1/3} h u^{-1/6} + \mathcal{O}_\kappa(u^{1/6})$$

$$= -\left(3^{1/3}(2\kappa)^{-1/3} f_0^{-1/3} + \mathcal{O}_\kappa(f_0^{1/3})\right),$$

which gives (b).

The expansion (c) results from the expression (2.3) of ϵ_0.

These asymptotics will also be compared to numerical results in the last section.

3. QUALITATIVE PROPERTIES OF THE INITIAL VALUE PROBLEM

The equations which give the superheating field for the half-space model are the GL equations (1.6)-(1.9), but, in order to avoid the numerical difficulties due to the conditions at infinity and to the very fast increase of A while f slowly varies, we shall instead treat a family of initial value problems associated to the GL equations. We try in this section to give some qualitative properties of this problem which will explain our choice in the numerical tests of the last section.

The system can be written as $Y' = F(Y, x)$, with

$$Y = (f, f', A, A'),$$

$$F(Y, x) = (f', \kappa^2(-f + f^3 + A^2 f), A', f^2 A) \quad x \in \,]0, T[\,,$$

for $T > 0$. We now give the initial conditions at $x = 0$. Two natural conditions $f'(0) = 0$ and $A'(0) = h$ are given by our problem. We add the two unknowns $f(0) = f_0$ and $A(0) = A_0$.

We get

$$f' = g \tag{3.1}$$

$$g' = \kappa^2[-f + f^3 + A^2 f] \tag{3.2}$$

$$A' = C \tag{3.3}$$

$$C' = f^2 A \tag{3.4}$$

with

$$f(0) = f_0, \quad g(0) = 0, \quad A(0) = A_0, \quad C(0) = h, \tag{3.5}$$

where f, g, A, C are in $C^1(\,]0,+T[\,)$, f_0 and $A_0 \in \mathbb{R}$. In the following, we shall denote Y_0 each initial condition of the form $(f_0, 0, A_0, h)$.

Because F is a C^1 function on $\mathbb{R}^4$, we know by standard results the existence, for every $Y_0 \in \mathbb{R}^4$, of a unique maximal solution $(Y; I_{max} = [0, T_{max}[\,)$ satisfying the differential system (3.1)-(3.5) on $]0, T_{max}[$ and the initial condition Y_0.

We are looking for solutions of the GL equations (1.6)-(1.9) on $]0, +\infty[$, we have then to study the existence of Y_0 such that $T_{max} = +\infty$ and such that

$$A \in H^2(\,]0,\infty[\,), \quad (1-f) \in H^2(\,]0,\infty[\,) \tag{3.6}$$

then, in particular

$$\lim_{x \to +\infty} f(x) = 1, \quad \lim_{x \to +\infty} A(x) = 0. \tag{3.7}$$

We have already recalled that a solution of the GL equations is such that $|f(x)| \leqslant 1$ for $x \in [0, +\infty[$. Let us give other properties of these solutions. The proofs of these results can be found in [5], [8] or [30].

PROPOSITION 3.1 : *Let (f, A) be a solution of (1.6)-(1.9), then :*
a) The function A is strictly increasing on $[0, +\infty[$, and we have :

$$0 \leqslant A'(x) \leqslant h. \tag{3.8}$$

b) If f is positive on $[0,\infty[$, then f is strictly increasing on $]0,\infty[$.
Moreover, we recall (see Remark 2.10) that, when such a global solution exists, (f, g, A, C) belongs to an hypersurface V_0 in $\mathbb{R}^4$ given (*cf.* (2.25)) by :

$$\kappa^{-2} g^2(x) + C^2(x) = \frac{1}{2}(1 - f^2(x))^2 + A^2(x) f^2(x).$$

Therefore we shall suppose in the following (and in our numerical computations of Subsection 4.2) that the initial condition Y_0 belongs to V_0, and consequently the initial conditions satisfy :

$$(a) \quad f'(0) = 0; \quad A'(0) = h \tag{3.9}$$

$$(b) \quad h^2 = \frac{1}{2}(1 - f_0^2)^2 + f_0^2 A_0^2.$$

We are looking for solutions such that f is positive and A negative, so that we shall suppose that

$$f_0 \in [0, 1] \quad \text{and} \quad A_0 \leqslant 0;$$

but, because the cases $f_0 = 0$, $f_0 = 1$ and $A_0 = 0$ are simpler limit cases, we shall in general assume that

$$f_0 \in \,]0, 1[\quad \text{and} \quad A_0 < 0 . \tag{3.10}$$

Furthermore, we shall restrict our study to the solutions of (3.1)-(3.5) such that f is nonnegative, although some results can be extended to some f which changes of sign in I_{max}.

Let us now partially study the solutions of the initial value problem (3.1)-(3.5). We first consider the stationary solutions.

Stationary solutions of (3.1)-(3.5)

We have

PROPOSITION 3.2 : *The only stationary solution of (3.1)-(3.5) satisfying (3.9), $f_0 \in [0, 1]$ and $A_0 \leq 0$, is the solution* $(1, 0, 0, 0)$; *it is an unstable solution.*

Proof: Stationary solutions are constant solutions such that $Y' = 0$. We get

$$(f = 0, A = m = \text{Const.}) \quad \text{or} \quad (A = 0, f = \pm 1) . \tag{3.11}$$

But, there are no 4-uplet $(f, f', A, A') = (0, 0, m, 0)$ satisfying (3.9) (and consequently the conservation law (2.25)) ; therefore the only stationary solution with $f_0 \geq 0$ is $(f, f', A, A') = (1, 0, 0, 0)$.

In order to show the instability of this solution, we have to study the linearized problem around the stationary solution $(1, 0, 0, 0)$, that is the system

$$V' = DF_Y((1, 0, 0, 0))\, V ,$$

where $DF_Y((1, 0, 0, 0))$ has $\lambda_{\pm} = \pm 1$, $\mu_{\pm} = \pm \sqrt{2}\,\kappa$ as eigenvalues. We then get a 2-dimensional stable manifold whose tangent space at $(1, 0, 0, 0)$ is spanned by $\left(1, -\sqrt{2}\,\kappa, 0, 0\right)$ and $\left(0, 0, 1, -\sqrt{2}\right)$ and a 2-dimensional unstable manifold whose tangent space is spanned by $\left(1, +\sqrt{2}\,\kappa, 0, 0\right)$ and $\left(0, 0, 1, +\sqrt{2}\right)$. The instability of the stationary solution $(1, 0, 0, 0)$ could explain some difficulties in the computation of a solution of (3.1)-(3.5) s.t. (3.6) and (3.9) are satisfied.

Variations of f and A

Let us write some partial results about the variations of the solutions f and A of the initial value problem (3.1)-(3.5) when the conditions (3.9) and (3.10) are satisfied. Under some additional assumptions, as the positivity of f, we try to analyze the different behaviors of the solution, and make more precise the classical result that a trajectory is either unbounded or converges towards a stationary solution.

The solutions of the GL equations are bounded solutions which are defined on $]0, +\infty[$; this is not the case for most of the solutions of the initial value problem. The two Lemmas 3.4 and 3.5 give, in particular, that $I_{\max}$ is finite or infinite, according only to the boundedness to f. But, let us first write a useful lemma

LEMMA 3.3 : *Let $(f, f', A, A' ; I_{\max})$ be a maximal solution of (3.1)-(3.5) satisfying (3.9)-(3.10).*

ii) If there exists $x_1 \in\ ]0, T_{\max}[$ such that $f(x_1) = 1$, then f is strictly increasing and convex on $]x_1, T_{\max}[$.

ii) If there exists $x_2 \in\ ]0, T_{\max}[$ such that $A(x_2) = 0$, then A is strictly increasing and convex on $]x_2, T_{\max}[$.

Proof : For i), let $\hat{x}_1$ be the smallest x_1 s.t. $f(x_1) = 1$, then, because f is not a constant function and $x \in\ ]0, +\infty[\ \to (1, 0, 0, 0)$ is a stationary solution, the Cauchy-Lipschitz Theorem implies that $f'(\hat{x}_1) > 0$. The equation $f''(x) = \kappa^2(-1 + f^2(x) + A^2(x))f(x)$ gives that $f''(x) \geqslant 0$ for $x \in\ ]\hat{x}_1, T_{\max}[$, and then $f'(x) \geqslant f'(\hat{x}_1) > 0$ on the same interval. Therefore, f is strictly increasing on $]x_1, T_{\max}[$.

The proof of ii) is analogous with the use of the equation $A'' = f^2 A$.

We can show

LEMMA 3.4 : *Let $(f, f', A, A' ; I_{\max})$ be a maximal solution of (3.1)-(3.5) satisfying (3.9)-(3.10).*

i) If both f and A are bounded on $I_{\max}$, then f' and A' are also bounded and $T_{\max} = +\infty$.

ii) If f is bounded on $I_{\max}$, then $T_{\max} = +\infty$.

Proof : For i), bounds for f' and A' result immediately from the conservation law given by (2.25) or

$$\kappa^{-2} f'^2(x) + A'^2(x) = A^2(x) f^2(x) + \frac{1}{2}(1 - f^2(x))^2 . \tag{3.12}$$

Now, if $T_{\max}$ was finite, a classical theorem says that $|f(x)| + |f'(x)| + |A(x)| + |A'(x)|$ tends to $+\infty$ as $x \to T_{\max}$. This gives a contradiction and then the first part of the lemma.

In order to prove the second part ii), we shall suppose that $T_{\max}$ is finite and get a contradiction.

If f is bounded, the equations (3.3) and (3.4) give that the pair $X = (A, A')$ is a solution of a linear equation which can be written as $X'(x) = M(x)\,X(x)$ where M is a bounded matrix on $[0, T_{max}[$. We get, using the norm ℓ^2 in $\mathbb{R}^4$ and the corresponding matrix norm

$$\|X'(x)\|_2 \leqslant \|M(x)\|_2 \,.\, \|X(x)\|_2 \leqslant C\|X(x)\|_2 \quad \text{for } x \in I_{max}\,,$$

(where C is a constant). Then, using a classical result about the derivative of the function $r(x) = \|X(x)\|_2^2$ for $x \in I_{max}$ and integrating, we get :

$$\|X(x)\|_2 \leqslant \|X(0)\|_2 \,.\, \exp Cx \quad \text{for } x \in I_{max}\,.$$

Therefore, the assumption that T_{max} is finite gives that A is bounded on I_{max}. But the part *i)* of the lemma says that $T_{max} = +\infty$ as soon as f and A are both bounded ; we get a contradiction and then $T_{max} = +\infty$.

LEMMA 3.5 : *Let $(f, f', A, A' ; I_{max})$ be a maximal solution of (3.1)-(3.5) satisfying (3.9)-(3.10). If there exists $x_1 \in I_{max}$ such that $f(x_1) = 1$, then T_{max} is finite and f tends to $+\infty$ as x tends to T_{max}.*

Proof : Let us first show that T_{max} is finite.

By multiplicating by f' and integrating the equations (3.1) and (3.2), we get for $\quad 0 \leqslant x < y < T_{max}$

$$f'^2(x) - f'^2(y) = \kappa^2\Big(-f^2(x) + \tfrac{1}{2}f^4(x)\Big) - \kappa^2\Big(-f^2(y) + \tfrac{1}{2}f^4(y)\Big)$$
$$+ 2\,\kappa^2 \int_y^x A^2(t)\,f(t)\,f'(t)\,dt\,. \tag{3.13}$$

Using Lemma 3.3 (i), we get that $f(x)\,f'(x) \geqslant 0$ for $x \in [x_1, T_{max}[$ with $f'(x_1) > 0$. Consequently, for $x \in\,]x_1, T_{max}[$

$$f'^2(x) \geqslant \frac{\kappa^2}{2}\,(f^2(x) - 1)^2 + C\,, \tag{3.14}$$

where

$$C = f'^2(x_1) - \frac{\kappa^2}{2}\,(f^2(x_1) - 1)^2 = f'^2(x_1) > 0\,. \tag{3.15}$$

Because f' is positive, we get, for $x \in\,]x_1, T_{max}[$,

$$f'(x) \geqslant \frac{\kappa}{\sqrt{2}}\,(f^2(x) - 1)\,;$$

then for $x \in \,]x_1, T_{max}[$

$$\frac{f'(x)}{f^2(x) - 1} \geq \frac{\kappa}{\sqrt{2}}$$

and for $x_1 < x \leq y < T_{max}$

$$\ln \left| \frac{f(y) - 1}{f(y) + 1} \right| \geq \sqrt{2}\, \kappa (y - x) + \ln \left| \frac{f(x) - 1}{f(x) + 1} \right| . \tag{3.16}$$

But $f(y) > 1$ for $y \in \,]x_1, T_{max}[$ and consequently the left hand side is negative. We get that T_{max} is finite.

The end of the proof of Lemma 3.5 is easy ; Lemma 3.4 (ii) implies that f is unbounded because T_{max} is finite, and Lemma 3.3(i) gives that f is strictly increasing on $]x_1, T_{max}[$; therefore $f(x)$ tends to $+\infty$ as x tends to T_{max}. We get in particular that the trajectory of the solution $(f, f', A, A' ; I_{max})$ is unbounded.

Remark 3.6 : The inequality (3.16) gives an interesting result for $f(x)$ as $x \to T_{max}$ when the assumptions of Lemma 3.5 are satisfied.

If we take the limit $y \to T_{max}$ in (3.16), we get for $x_1 < x < T_{max}$:

$$\sqrt{2}\, \kappa (T_{max} - x) \leq - \ln \left| \frac{f(x) - 1}{f(x) + 1} \right| ;$$

then, for every $\epsilon > 0$, there exists $\eta_1 > 0$ such that for $0 < T_{max} - x \leq \eta_1$:

$$(T_{max} - x) f(x) \leq (1 + \epsilon)\, 2^{1/2} \kappa^{-1} . \tag{3.17}$$

If we add, to the hypothesis of Lemma 3.5, the assumption that A is bounded on I_{max}, we get for f an analogous lower bound. This is the object of the following lemma.

LEMMA 3.7 : *Let $(f, f', A, A' ; I_{max})$ be a maximal solution of (3.1)-(3.5) satisfying (3.9)-(3.10) and let us suppose that A is bounded on I_{max}. If there exists $x_1 \in I_{max}$ such that $f(x_1) = 1$ then :*

i) *for every $\epsilon > 0$, there exists $\eta > 0$ such that for $0 < |T_{max} - x| \leq \eta$:*

$$\left| f(x) - \frac{2^{1/2}}{\kappa (T_{max} - x)} \right| \leq \epsilon \frac{2^{1/2}}{\kappa (T_{max} - x)} ;$$

ii) *both A and A' tend to 0 as $x \to T_{max}$ and*

$$A(x) = \mathcal{O}((T_{max} - x)^{\alpha_0}) \text{ as } x \to T_{max} , \quad \text{with} \quad \alpha_0 = C\kappa^{-1} + \mathcal{O}(1) .$$

Proof : The results of Lemma 3.5 and of Remark 3.6 remain true ; we shall get i) using an analogous proof and the conservation law (2.25).

Proof of i).

Let us first give an equivalent for f as $x \to T_{\max}$.

Let M be a constant s.t. $|A(x)| \leqslant M$ for $x \in I_{\max}$; we can easily suppose that $M \geqslant 2$, then, using the conservation law (2.25), we get :

$$\forall x \in I_{\max} \quad \kappa^{-2} f'^2(x) \leqslant f^2(x) M^2 + \tfrac{1}{2}(1 - f^2(x))^2$$
$$\leqslant \tfrac{1}{2}(f^2(x) + M^2 - 1)^2 .$$

Therefore, using that $M > 1$ and f' is positive for $x > x_1$, we get :

$$0 < \kappa^{-1} f'(x) \leqslant 2^{-1/2}(f^2(x) + M^2 - 1) ;$$

and then, by integrating over $[x, y]$, with $x_1 < x < y < T_{\max}$:

$$\tan^{-1}\left(\frac{f(y)}{\sqrt{M^2 - 1}}\right) \leqslant 2^{-1/2} \kappa \sqrt{M^2 - 1}\,(y - x) + \tan^{-1}\left(\frac{f(y)}{\sqrt{M^2 - 1}}\right) .$$

If we take the limit $y \to T_{\max}$, we get for $x_1 < x < T_{\max}$:

$$f(x) \geqslant \sqrt{M^2 - 1} \tan\left(\frac{\pi}{2} - 2^{-1/2} \kappa \sqrt{M^2 - 1}\,(T_{\max} - x)\right) ;$$

then, for every $\epsilon > 0$, there exists $\eta_2 > 0$ such that for $0 < T_{\max} - x \leqslant \eta_2$:

$$(T_{\max} - x) f(x) \geqslant (1 - \epsilon)\, 2^{1/2} \kappa^{-1} . \tag{3.18}$$

Using (3.17) and $\eta = \inf\{\eta_1, \eta_2\}$, we get i) ; and in particular :

$$f(x) = \mathcal{O}((T_{\max} - x)^{-1}) \quad \text{as } x \to T_{\max} .$$

ii) Let us show that A tends to 0 as $x \to T_{\max}$.

By integrating the equation $-A'' + f^2 A = 0$ with the initial condition $A'(0) = h$ over $[0, x]$ with $x \in\,]0, T_{\max}[$, we get :

$$A'(x) = h + \int_0^x f^2(t) A(t)\, dt ; \tag{3.19}$$

with A negative and A' positive on $[0, T_{\max}[$ (A is increasing) ; moreover A', positive and decreasing on $I_{\max}$ admits a non-negative limit l as $x \to T_{\max}$.

Now, it results from (3.18) that $f(x) \geqslant \frac{C}{T_{max} - x}$ when $x \to T_{max}$; therefore, the integral in (3.19) is only convergent, as $x \to T_{max}$, when A tends to $m = 0$; using that, in the opposite case (that is $m < 0$) A' cannot have a limit as $x \to T_{max}$, we get a contradiction and then that $m = 0$.

For A', integrating by parts

$$\int_0^x \frac{A(t)\,dt}{(T_{max} - t)^2} = -\frac{A(T_{max}) - A(x)}{T_{max} - x} - \frac{A(0)}{T_{max}} - \int_0^x \frac{A'(t)\,dt}{T_{max} - t},$$

we get that the limit of A' as $x \to T_{max}$ is also $l = 0$.

The behavior of A as $x \to T_{max}$ follows from standard technics on ODE by reducting to a Ricatti equation.

The next lemma gives informations about the local extrema for A when f is supposed to be non-negative on I_{max} ; this will help us to classify the solutions of the initial value problem with a view to our numerical computations. We first remark that if $f_0 > 0$, thanks to the Cauchy-Lipschitz Theorem, the assumption $f \geqslant 0$ on I_{max} implies that f is strictly positive on this interval.

LEMMA 3.8 : *Let* $(f, f', A, A'; I_{max})$ *be a maximal solution of (3.1)-(3.5) satisfying (3.9)-(3.10). If f is non-negative on* I_{max}, *then A has, in* $]0, T_{max}[$, *at most one local maximum which is strictly negative and no local minimum.*

Proof : Let us show that every local maximum of A in $]0, T_{max}[$ is strictly negative (see in [5] the study of the GL equations in a bounded interval with boundary conditions). Let $x_0 \in\ ]0, T_{max}[$ be a point where A is locally maximal, then

$$A'(x_0) = 0 \quad \text{and} \quad A''(x_0) \leqslant 0 .$$

The equations (3.3) and (3.4) give then

$$f^2(x_0)\,A(x_0) \leqslant 0 ,$$

and using the assumption $f > 0$, we get $A(x_0) \leqslant 0$.

But according to the Cauchy-Lipschitz Theorem, we get $A(x_0) < 0$.

Similarly we get that a local minimum satisfies $A(x_0) > 0$; but with $A(0) < 0$, this implies the existence of a positive local maximum which is excluded.

Moreover, the existence of two negative local maxima implies the existence of a negative local minimum which is again excluded. The lemma is proved.

As a first consequence, we get for A the following lemma which has to be compared with Lemma 3.3.

LEMMA 3.9 : *Let* $(f, f', A, A'; I_{\max})$ *be a maximal solution of (3.1)-(3.5) satisfying (3.9)-(3.10) and such that f is non-negative on* $I_{\max}$. *If there exists* $x_3 \in \,]0, T_{\max}[$ *such that* $A'(x_3) = 0$, *then A and A′ are strictly decreasing on* $]x_3, T_{\max}[$, *and A is negative on* $I_{\max}$.

Proof: We first observe that $A''(x_3)$ is different from 0, because $-A'' + f^2 A = 0$ on $I_{\max}$. This proves that A has a non degenerate extremum at x_3, and according to Lemma 3.8, this is a local maximum with $A(x_3) < 0$. For $x > x_3$, we have consequently $A(x) < 0$ and then $A''(x) < 0$. Therefore A and A' are strictly decreasing on $]x_3, T_{\max}[$ and A is negative on $I_{\max}$.

The next lemma completes Lemma 3.4 (i) when f is non-negative :

LEMMA 3.10 : *Let* $(f, f', A, A'; I_{\max})$ *be a maximal solution of (3.1)-(3.5) satisfying (3.9)-(3.10) and such that f and A are bounded and f is positive on* $I_{\max}$, *then* (f, f', A, A') *is a solution of the GL equations on* $]0, +\infty[$.

Proof: We shall use several steps.

Step 1 : $T_{\max} = +\infty$ and f' and A' are bounded on $]0, +\infty[$.

This is just Lemma 3.4 (i) because f and A are bounded on $I_{\max}$.

Step 2 : A is negative and strictly increasing on $]0, +\infty[$.

We proceed by contradiction. If A is not negative on the whole interval $]0, +\infty[$, there exists $x_2 \in \,]0, +\infty[$ such that $A(x_2) = 0$; then Lemma 3.9(i) gives that A is strictly increasing on $]x_2, +\infty[$ and then unbounded on $I_{\max}$ because $T_{\max}$ is infinite. We get a contradiction, and that A is strictly negative on $[0, +\infty[$.

Using an analogous proof we get that A' is strictly positive on $[0, +\infty[$; if it is not the case, there exists $x_3 > 0$ such that $A'(x_3) = 0$, and Lemma 3.9(ii) implies that $A' < 0$ on $]x_3, +\infty[$; therefore A is strictly decreasing on that interval, and because $T_{\max} = +\infty$, A tends to $-\infty$ as $x \to +\infty$, which gives also a contradiction.

Consequently, A is strictly increasing and negative on $[0, +\infty[$.

Step 3 : f is an increasing function on $[0, +\infty[$.

It is sufficient to show that f' is non-negative on $[0, +\infty[$ We proceed also by contradiction. Let us suppose that there exists $y_0 > 0$ such that $f'(y_0) < 0$, then we distinguish two cases :

- a) f' admits at least a local minimum,
- b) f' has no minimum but is decreasing as x tends to $+\infty$.

Case a) : We assume that there exists $x_0 > 0$ where the function $g = f'$ is locally minimal. We have

$$f''(x_0) = 0 \quad \text{with} \quad f'(x_0) < 0 \,, \tag{3.20}$$

because $f'(x_0) \leqslant f'(y_0) < 0$. Therefore, using the equation (3.2), we get :

$$-1 + f^2(x_0) + A^2(x_0) = 0 . \tag{3.21}$$

and then, using that f is strictly positive

$$3 f^2(x_0) - 1 + A^2(x_0) = 2 f^2(x_0) > 0 . \tag{3.22}$$

Let us consider the equation satisfied by g which is obtained by derivation of the equation (3.2), that is

$$-\kappa^{-2} g'' + (3 f^2 - 1 + A^2)\, g = -2 AA' f . \tag{3.23}$$

At the point x_0, we have :

$$g''(x_0) \geqslant 0 ; \quad -A(x_0) A'(x_0) f(x_0) \geqslant 0 ; \quad g(x_0) = f'(x_0) < 0 ,$$

so that we get a contradiction with (3.22).

Consequently, f' cannot have any local minimum on $]0, +\infty[$, and the assumption that there exists $x_3 > 0$ s.t. $f'(x_3) < 0$ implies that the case b) holds.

Case b) : We assume now that f' is decreasing as $x \to +\infty$.

Because it is also bounded, f' admits a limit, denoted by β, as x tends to $+\infty$. We get that $\beta = 0$ because for x large enough $f(x+1) - f(x) = f'(\xi) \in [\beta, \beta + \epsilon]$ (where $\xi \in\,]x, x+1[$), so that, if $\beta \neq 0$, f does not stay bounded and we have again a contradiction.

Therefore f' is a non-negative function on $]0, +\infty[$ and f is increasing on $]0, +\infty[$.

Step 4 : The limit m of A is 0 as $x \to +\infty$.

Because f is a bounded increasing function, it admits a limit α as x tends to $+\infty$. On an other hand, $A \leqslant 0$ implies that $A'' \leqslant 0$ on $[0, +\infty[$, so that A' is decreasing and bounded, and admits also a limit l as x tends to $+\infty$. Let us show that $l = 0$; this limit is non-negative because A is increasing, and moreover, for every $x \in\,]0, +\infty[$, $A(x+1) - A(x) = A'(\xi) \geqslant l$ with $\xi \in\,]x, x+1[$, so that, if $l > 0$, A cannot have a limit as x tends to $+\infty$.

Using now the conservation law (3.12), we get that f' has also a limit as x tends to $+\infty$. Let β be the limit of f'; β is non-negative because f is increasing. Let us show that $\beta = 0$. We use again the relation $f(x+1) - f(x) = f'(\xi)$ with $\xi \in\,]x, x+1[$ and we get $f'(\xi) \geqslant \beta - \epsilon$ for x large enough, so that β cannot be strictly positive.

At the limit, when x tends to $+\infty$ in (3.12), we get :

$$m^2 \alpha^2 + \frac{1}{2}(1 - \alpha^2)^2 = 0 .$$

Therefore :

$$m = 0 \quad \text{and} \quad \alpha = 1 ,$$

and (f, f', A, A') is a solution of the GL equations.

As a consequence of the preceding study, we have :

THEOREM 3.11 : *Let $(f, f', A, A'; I_{\max})$ be a maximal solution of (3.1)-(3.5) satisfying (3.9)-(3.10). If f is positive on $I_{\max}$, then A has one of the four following behaviors :*

(α) A is strictly increasing and becomes strictly positive,

(β) (f, A) is a solution of the GL equations on $]0, +\infty[$,

(γ) A is a concave function and A' becomes strictly negative,

(δ) A is strictly increasing, A' is strictly decreasing, the both tend to the finite limit 0 as $x \to T_{\max}$, where $T_{\max}$ is finite, and f tends to $+\infty$ as $x \to T_{\max}$.

Proof : We distinguish several cases.

i) There exists $x_1 > 0$ such that $f(x_1) = 1$.

Then, using Lemma 3.5, we get that $T_{\max}$ is finite and f tends to $+\infty$ as $x \to T_{\max}$. Now, Lemma 3.8 gives that :

• either A admits a local maximum and we get the case (γ),

• or A is strictly increasing on $I_{\max}$ and we get once again two possible cases according to the existence or not of a point x_2 such that $A(x_2) = 0$; we get indeed :

— either the case (α),

— or A admits a finite limit m such that $m \leqslant 0$ as $x \to T_{\max}$. Then Lemma 3.7 shows that $m = 0$ and that A' tends also to the limit 0. We get the case (δ).

ii) For every $x \in I_{\max}$ then $f(x) < 1$:

Lemma 3.4(ii) implies that $T_{\max} = +\infty$. Now,

• if A is unbounded on $]0, +\infty[$, then, from Lemma 3.8, A satisfies one of the two cases (α) or (γ) (according also to the existence or not of x_2 s.t. $(A(x_2) = 0)$.

• if A is bounded on $]0, +\infty[$, then we get the case (β) using Lemma 3.10.

We would be glad to characterize the initial conditions which lead to each of these behaviors given by Theorem 3.11.

Remark 3.12 : Let us remark that, in the two cases (α) and (γ), f can be bounded or unbounded. When f is unbounded, we get from Lemma 3.5 that T_{max} is finite and f tends to $+\infty$. When f is bounded, we get from Lemma 3.4(ii) that $T_{max} = +\infty$.

Let us improve this last result as follows.

If the maximal solution $(f, f', A, A'; I_{max})$ satisfies (3.9)-(3.10), if f is bounded and non-negative, and if A is unbounded on I_{max}, then f tends to 0 as x tends to $+\infty$.

Proof: Because A is not bounded, it results from Lemma 3.9(i) or (ii) (according to the sign of A as $x \to +\infty$) that there exists $x_4 > 0$ such that $A^2(x) \geqslant 1$ for every $x \in [x_4, +\infty[$. Using the relation $f''(x) = \kappa^2(-1 + A^2(x) + f^2(x))\ f(x)$, we get that $f'' > 0$ on $[x_4, +\infty[$, so that f is convex on that interval and because it is also bounded, it admits a limit α as $x \to +\infty$.

On an other hand, $(-1 + A^2(x) + f^2(x))$ tends to $+\infty$ as $x \to +\infty$, so that the limit α of f is necessarily 0, otherwise f'' would tend to $+\infty$ as $x \to +\infty$ and f would not be bounded.

In Subsection 4.2, we define numerical tests for getting a solution of the GL-equations. They use Theorem 3.11, but also some properties of monotonicity for A as function of h, when f_0 remains constant, which are observed in the computations.

4. NUMERICAL COMPUTATIONS OF THE SUPERHEATING FIELD, COMPARISON WITH THE PHYSICAL LITERATURE

We try to compute, in this section, numerical solutions of the limit problem (1.6)-(1.9) for weak values of the parameter κ and for various values of the parameter h. We try to have sufficiently precise computations in order to analyze possible two terms asymptotics of the superheating field H_{sh} for this half-space problem and to compare the results that we obtain with the different formulas or numerical computations which have appeared in the literature.

Let us first recall the different results on the superheating field given in the physical literature.

4.1. The superheating field in the physical literature

Different formulas for the superheating field are given in the literature and the purpose of this subsection is to analyze the « proofs » and the numerical results. We emphasize that we are not comparing with experimental results. We only try to analyze the results given by the GL equations, in particular, as κ tends to 0.

The first « analytic » formula was proposed by the Orsay group in [26] :

$$H_{sh}/H_c \approx 2^{-1/4}\kappa^{-1/2} \tag{4.1}$$

where

$$2^{-1/4} \approx 0.8409 .$$

An earlier result was given by V. L. Ginzburg [21]. Starting of some homogeneity argument, the author assumes that asymptotically

$$H_{sh}/H_c \approx C\kappa^{-1/2} \tag{4.2}$$

and compute the constant for $\kappa = 0.02$. He obtains in this way the formula :

$$H_{sh}/H_c \approx 0.89 \,.\, \kappa^{-1/2} . \tag{4.3}$$

In 1973, Parr and Feder [28] propose on the basis of numerical computations the following asymptotics :

$$H_{sh}/H_c \approx \kappa^{-1/2}2^{-1/4}(1 + 0.535 \,.\, \kappa) , \tag{4.4}$$

with the comment that this approximation is good for $\kappa < 0.8$. This gives for example for the constant C in equation (4.2),

$$C = 1.011 \,.\, 2^{-1/4} \quad \text{when} \quad \kappa = 0.02$$
$$C = 1.16 \,.\, 2^{-1/4} \quad \text{when} \quad \kappa = 0.3 .$$

In [27] in 1976, Hugo Parr produces by heuristic analytic arguments the following two terms asymptotic formula :

$$H_{sh}/H_c \approx \kappa^{-1/2}2^{-1/4}\left(1 + \left(\frac{15\sqrt{2}}{32}\right)\kappa\right). \tag{4.5}$$

Let us mention that $\left(15\sqrt{2}/32\right) \approx 0.6629$.

We shall compare with the numerical results given by Fink and all in [17]. We have actually not very well understood if their results correspond to a direct computation on the GL-system or if they are obtained through an approximate analytical formula. The results are the following :

$$\begin{array}{lllllll} \kappa & 10^{-3} & 3.10^{-3} & 10^{-2} & 3.10^{-2} & 10^{-1} & 3.10^{-1} \\ H_{sh}/H_c & 26.71 & 15.47 & 8.496 & 4.952 & 2.828 & 1.809 . \end{array} \tag{4.6}$$

These authors propose also an approximate formula for κ near 1, but $\kappa < 1$

$$H_{sh}/H_c \approx \kappa^{-1/2} 2^{-1/4}(1 + 0\,658\,\kappa - 0\,237\,\kappa^2 + 0\,009\,\kappa^3) \qquad (4\,7)$$

The coefficients of (4 7) are actually introduced in order to get a very good approximation for the relatively large κ because the correction is only significative for $\kappa \gg 10^{-2}$ This formula cannot apparently be considered as an asymptotic formula in the mathematical sense, but it is probably more an interpolation formula calculated in order to fit with the numerical results

Let us compare these different results in several tables We introduce

$$\Delta = 2^{1/4}\,\kappa^{1/2}\left(\frac{H_{sh}}{H_c}\right) - 1\,, \quad \text{and compute } \Delta/\kappa$$

We recall that Δ gives the difference with the formula (4 1), and that $\Delta/\kappa \approx 0\,6629$ in the Parr's formula (4 5) In the following tables the different numerical values have been calculated from the formulas or results referenced in column 1 with the notations « Fink (a) » refers to the table (4 6), « Fink (b) » to the formula (4 7), « BoHe » to the formula (2 19) and « Parr » to (4 5)

Comparison of Δ from these various formulas

κ	10^{-3}	$3\,10^{-3}$	10^{-2}	$3\,10^{-2}$	10^{-1}	$3\,10^{-1}$
Fink (a)	0 0045	0 0076	0 0103	0 0200	0 0638	0 1782
Fink (b)	0 00066	0 00198	0 0066	0 0195	0 064	0 176
BoHe	0 0031	0 0077	0 021	0 046	0 10	0 16
Parr	0 00066	0 002	0 0066	0 020	0 066	0 20

Comparison of Δ/κ

κ	10^{-3}	$3\,10^{-3}$	10^{-2}	$3\,10^{-2}$	10^{-1}	$3\,10^{-1}$
Fink (a)	4 5	2 53	1 03	0 66	0 63	0 594
Fink (b)	0 66	0 66	0 66	0 65	0 64	0 59
BoHe	3 05	2 56	2 035	1 55	1 01	0 53

All these formulas are relatively good for Δ in absolute value, but the analysis of Δ/κ, for κ small, shows strong divergence between the different computations The formula (4 1) of the Orsay group appears as a good asymptotics when κ tends to 0, but the second term in the expansion of H Parr (4 5) fits only with « Fink (b) » (or (4 6)) when κ is small and with « Fink (a) » (or (4 7)) when κ is near $3\,10^{-2}$ On an other hand, our formula (2 19) does not agree very well with the other different results

But our main remark is that the numerical values obtained for small κ are not sufficiently accurate in order to guess a second term for the asymptotics. This remark leads us to undertake a numerical study of this problem. This is the object of the remainder of this section.

4.2. A numerical study of the superheating field

The numerical method that we shall use in order to compute a solution of the half-space model, is a shooting method on the family of initial value problems (3.1)-(3.5), with the additional conditions (3.7).

Each initial value problem is solved by a semi-implicit Runge-Kutta method (of order 3 with 2 intermediate steps) which is an A-stable method (see M. Crouzeix [15] where this numerical scheme is studied ; see also [16]). Such a method is used to solve the so called stiff problems which are very sensitive to a small variation of the initial conditions. This will be the case in our problem because we are looking for trajectories which tend to the unstable stationary solution $(1, 0, 0, 0)$ as x tends to ∞.

The Runge-Kutta method with a variable stepsize that we have chosen is not a symplectic integration method, but this method gives satisfactory results in our numerical computations of the superheating field (see Subsection 4.2.2) ; in particular, we verify *a posteriori* that the conservation law (2.25) is satisfied up to a sufficiently small error in an interval large enough for giving all the informations that we are looking for.

4.2.1. *The numerical scheme*

Let us describe this numerical scheme. If Y_0 is a prescribed initial condition, we want to compute numerical approximations for the solution Y on an ordered set of points x_i, $\{i = 1, ..., n\}$ of the interval $]0, T_{\max}[$. Let us suppose that Y_i is a computed approximation of :

$$Y(x_i) = (f(x_i), f'(x_i), A(x_i), A'(x_i)) \text{ at a point } x_i \geqslant 0 .$$

Let H_i be a steplength and $x_{i+1} = x_i + H_i$, then $Y(x_{i+1})$ will be approximated by the solution Y_{i+1} of the system :

$$\begin{aligned} Y_{i,1} &= Y_i + \tau H_i F(Y_{i,1}, x_{i,1}) \\ Y_{i,2} &= Y_i + \tau H_i F(Y_{i,2}, x_{i,2}) - \left(\frac{1}{\sqrt{3}}\right) H_i F(Y_{i,1}, x_{i,1}) \qquad (4.8) \\ Y_{i+1} &= Y_i + \frac{1}{2} H_i \cdot [F(Y_{i,1}, x_{i,1}) + F(Y_{i,2}, x_{i,2})] , \end{aligned}$$

where :

$$\tau = \frac{1}{2}\left(1 + \frac{1}{\sqrt{3}}\right),$$

$$x_{i,1} = x_i + \tau H_i, \tag{4.9}$$

$$x_{i,2} = x_i + (1 - \tau) H_i .$$

The two first equations in (4.8) define $Y_{i,1}$ and $Y_{i,2}$ implicitely ; we must solve them using iterative methods.

The steplength H_i will be calculated at each step, using a comparison of the computations at each point with two different steplengths.

According to Section 3, an initial condition Y_0 will always be chosen such that (3.9) and (3.10) are satisfied.

4.2.2. *Numerical tests*

In order to select approximations of the initial condition f_0 and of the exterior magnetic field h which lead to an approximate solution of the GL equations, we choose some rules which will allow us to interpret our numerical computations.

According to the theoretical results given in Lemmas 3.3, 3.5 and 3.9 and to a lot of tests performed from various values of all the parameters, we consider that a computed trajectory cannot give a solution of the GL equations as soon as one of the following conditions is fulfilled (up to a given error) : A crosses the value 0, A' crosses the value 0, f one of the values 1 or 0. Consequently, we have set up some numerical tests which stop the iterations when one of these conditions is fulfilled. We then get a lot of different cases that we have to classify ; but, our numerical results will confirm that we shall not meet other cases than the four given by Theorem 3.11.

a) Definitions

Let (x_i) be the sequence of points given, as in Subsection 4.2.1, by

$$x_{i+1} = x_i + H_i \quad \text{for } i \in \mathbb{N} ,$$

then a computed solution of (3.1)-(3.5) is a sequence $Y^{ap} = (Y_i)_{(i)}$ in $\mathbb{R}^4$ with $Y_i = (f_i, g_i, A_i, C_i)$, where f_i, g_i, A_i, C_i are approximations of $f(x_i)$, $f'(x_i)$, $A(x_i)$, $A'(x_i)$.

By analogy with the theoretical results of Section 3 and in particular with Theorem 3.11, we choose the following definitions :

DEFINITION 4.1 : *Let* $\epsilon_1 > 0$, $\epsilon_2 > 0$, $\epsilon_3 > 0$ *and* $\epsilon_4 > 0$ *be four small positive constants.*

A computed solution Y^{ap} of (3.1)-(3.5) is called of **type** (α^{ap}) if there exists $n \in \mathbb{N}$ s.t.

$$A_n \geq \epsilon_1 \;;\quad A_i < \epsilon_1 \quad \text{for } i = 0, \dots, n-1 \;;$$

$$C_i > -\epsilon_2 \quad \text{for } i = 0, \dots, n \;;$$

$$f_i \in \;]-\epsilon_3, 1+\epsilon_4[\quad \text{for } i = 0, \dots, n\,.$$

A computed solution Y^{ap} of (3.1)-(3.5) is called of **type** (β^{ap}) if there exists $n \in \mathbb{N}$ s.t.

$$|f_n - 1| \leq \epsilon_4, \quad f_i \in \;]-\epsilon_3, 1+\epsilon_4[\quad \text{for} \quad i = 0, \dots, n-1 \;;$$

$$A_i < \epsilon_1 \quad \text{for } i = 0, \dots, n \;;$$

$$C_i > -\epsilon_2 \quad \text{for } i = 0, \dots, n\,.$$

A computed solution Y^{ap} of (3.1)-(3.5) is called of **type** (γ^{ap}) if there exists $n \in \mathbb{N}$ s.t.

$$C_n \leq -\epsilon_2 \quad C_i > -\epsilon_2 \quad \text{for } i = 0, \dots, n-1 \;;$$

$$A_i < \epsilon_1 \quad \text{for } i = 0, \dots, n \;;$$

$$f_i \in \;]-\epsilon_3, 1+\epsilon_4[\quad \text{for } i = 0, \dots, n\,.$$

A computed solution Y^{ap} of (3.1)-(3.5) is called of **type** (δ^{ap}) if there exists $n \in \mathbb{N}$ s.t.

$$f_n \geq 1+\epsilon_4 \quad f_i \in \;]-\epsilon_3, 1+\epsilon_4[\quad \text{for } i = 0, \dots, n-1 \;;$$

$$A_i < \epsilon_1 \quad \text{for } i = 0, \dots, n \;;$$

$$C_i > -\epsilon_2 \quad \text{for } i = 0, \dots, n\,.$$

A computed Y^{ap} of (3.1)-(3.5) of type (β^{ap}) will be an approximation of a solution of the GL equations on the half-space.

b) Tests when κ and f_0 are fixed

We first test the method described in Subsection 4.2.1 with various values of h, when f_0 is fixed (for example, $f_0 = 0.8$ and $\kappa = 0.003$). Here, we recall that when h and f_0 are given, A_0 is determined by (3.9)(b) and $A_0 < 0$.

We observe only two different behaviors for the computed Y^{ap} ; Y^{ap} appears to be of *type* (α^{ap}) for small h and of *type* (γ^{ap}) for large h (*see fig. 1*).

The computed solution f has always the same behavior. It is given by an increasing sequence f_i, and, if we do not stop the iterations when we have

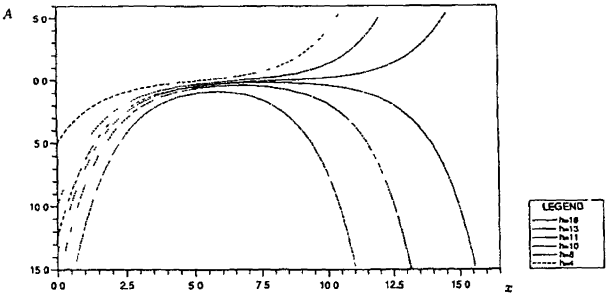

Figure 1. — The computed solutions A of the IVP when $\kappa = 0\,003$ and $f_0 = 0\,8$

found a value n of the index i which allows us to determine the type of a computed solution, then the sequence f_i crosses the value 1 more or less quickly according to the value of h (*see fig. 2*).

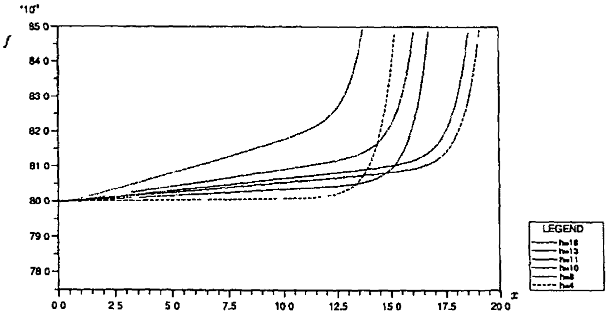

Figure 2. — The computed solutions f of the IVP when $\kappa = 0\,003$ and $f_0 = 0\,8$

But we get that $f_i \in \,]0, 1[$ for $i \in \{0, 1, \ldots, n\}$ with n large enough so that one of the type (α^{ap}) or (γ^{ap}) for the computed solution can be determined. In particular, we never find solutions of *type* (β^{ap}), neither solutions of *type* (δ^{ap}).

Let us consider, for some given $f_0 \in \,]0, 1[$ (for example $f_0 = 0.8$) the curve $h \to x_A(h)$ where $x_A(h)$ is, when it exists, the unique solution of $A(x_A(h)) = 0$ and where $A(x)$ is a solution of the IVP. We observe that this curve can be computed on an interval $[h_{inf}, h^c[$ (with $h_{inf} = 2^{-1}(1 - f_0^2)^2$ corresponding to $A_0 = 0$) and that it is increasing and tends to $+\infty$ as h tends to the critical value h^c.

If we consider, now, the curve $h \to x_{A'}(h)$ where $x_{A'}(h)$ is the unique solution of $A'(x_{A'}(h)) = 0$, we observe that this curve can be computed for every $h > h^c$ (with the same critical value h^c as before), and that $x_{A'}(h)$ tends to $+\infty$ as $h \to h^c$ with $h > h^c$ (*see fig. 3*).

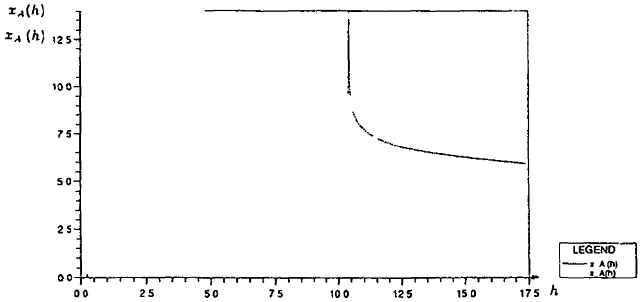

Figure 3 — The curves $x_A(h)$ and $x_A\ (h)$ when κ = 0 003 and f_0 = *0 8*

This particular behavior of the roots of $A(x) = 0$ suggests that there does not exist any trajectory such that $I_{\max}$ is bounded and A tends to 0 as $x \to T_{\max}$ The behavior of the roots of $A'(h) = 0$ confirms this idea This means that there is a little chance for the existence of a solution of *type* (δ^{ap})

On an other hand, the behavior of the two curves $x_A(h)$ and $x_A\,(h)$ lead us to think that the critical value h^c is associated to a solution of *type* (β^{ap}) This means that, with the assumption that these properties can be generalized to others values of f_0 and κ, we can determine closed bounds for a value of h such that the corresponding solution (f, f', A, A') satisfies the conditions (3 7) This leads us to propose, as in the preceding example, the following rule

Rule R_1

If, for some $f_0 \in\ ]0, 1[$, there exist two values h_1 and h_2 of h such that for one of them the computed solution Y^{ap} is of type (α^{ap}) and, for the other one, Y^{ap} is of type (γ^{ap}), then there exists a critical value h^c between h_1 and h_2 such that the corresponding solution is of type (β^{ap})

At last, and because the two different behaviors of a trajectory (that is A crosses the value 0 or A' crosses 0) can easily be determined, a *dichotomy method* will allow us to get a good approximation of the critical h_c

c) κ and h are fixed

We shall say that f_0^c is a critical value of f_0 if the computed Y^{ap}'s changes of type when f_0 crosses the value f_0^c

Now, if we keep a fixed h while f_0 varies, we observe for h small enough one or two critical values of f_0, and for large h no critical value of f_0

d) Using rules

From the preceding studies, we propose the following rules that we shall use to interprete our numerical computations :

Rule R_1' (instead of Rule R_1) :

If, for some $h > 0$, *there exist two initial conditions* f_0^1 *and* f_0^2 *of* f_0 *in* $]0, 1[$ *such that, for one of them,* Y^{ap} *is of type* (α^{ap}) *and, for the other,* Y^{ap} *is of type* (γ^{ap}), *then there exists a critical value* f_0^c *between* f_0^1 *and* f_0^2 *such that the corresponding solution is of type* (β^{ap}).

The numerical computations use a bisection method in order to get the critical values f_0^c.

Let us remark that a value of h satisfying the assumptions of the Rule R_1' gives a lower bound for the superheating field $H_{sh}(\kappa, \infty)$. For small values of h it is easy to find such f_0^1 and f_0^2, but this is more difficult for h near $H_{sh}(\kappa, \infty)$ because there exist two critical values of f_0 near each other, and f_0^1 and f_0^2 have to separate them (*see fig. 4*).

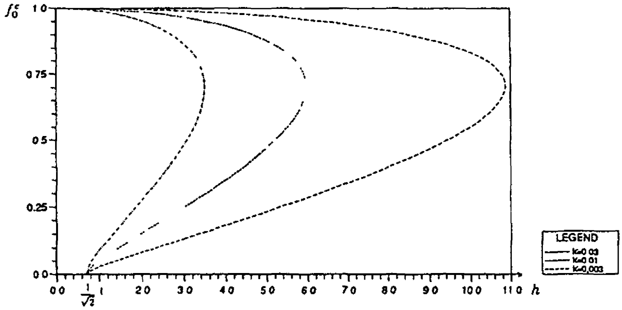

Figure 4. — The critical values f_0^c **as function of** h **for various** κ

On an other hand, it is not so easy to get an upper bound for $H_{sh}(\kappa, \infty)$, because we have to be sure that A has always the same sign for any f_0. In our computations, we define a steplength δf_0 small enough and we study the behavior of A for every $f_0 = p\,\delta f_0$ such that $p \in \mathbb{N}$ and $f_0 \in \,]0, 1[$. Then,

Rule R_2 :

If the computed Y^{ap}'s *keep the same type on all the points of the set* $S_{f_0} = \{f_0 = p\,\delta f_0\,;\, p \in \mathbb{N}\} \cap \,]0, 1[$, *we decide that* $h > H_{sh}(\kappa, \infty)$.

Assuming the Rules R_1' and R_2, a bisection method on the parameter h will give the *greatest field belonging to a prescribed interval,* for which there exists computed (f, A) such that the asymptotic conditions (3.7) are numerically satisfied.

e) Numerical results

Figure 4 gives the computed critical solutions f_0^c as function of h for various κ. We get a curve of « maximal » solutions starting from $f_0 = 1$, which is defined for $h \in \,]\epsilon, H_{sh}^c]$, with $\epsilon > 0$ (and for example $H_{sh}^c \approx 10.87758$ when $\kappa = 0.003$), and a curve of « minimal » solutions starting from $f_0 = 0$, defined for $h \in \,]\frac{1}{\sqrt{2}}\,; H_{sh}^c]$.

We get in particular that the curve $f_0 \to h = h(f_0)$ has a maximum at $h = H_{sh}^c$ which suggests the existence of a superheating field.

Figure 5 gives the corresponding $A^c(0)$ as function of h.

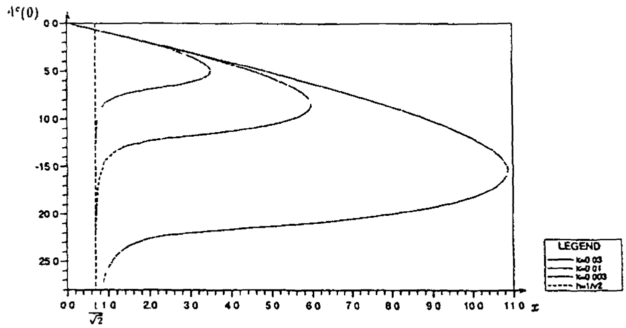

Figure 5. — The corresponding $A^c(0)$ as function of h.

We observe that, for initial conditions such that (f_0, h) belongs to the domain limited by the curve of the maximal solutions, the curve of the minimal solutions and the axis $h = 0$, then a computed solution is always of type (α^{ap}), while a computed solution is of type (γ^{ap}) in the exterior domain.

Remark 4.2 : Our numerical computations show in particular that when f_0 tends to 0, $h(f_0)$ tends to $1/\sqrt{2}$ and $A(0)$ tends to $-\infty$. We recall (see Lemma 2.12) that the same property was observed for the approximate model in Section 2.

Figure 6 shows the computed solutions $f(x)$ when $h = H_{sh}^c$ and x small, for various values of κ. Figure 7 gives the corresponding $A(x)$.

We remark that the results are very sensitive to the accuracy of the initial value f_0 so that on larger intervals than those of these two figures, we observe a sudden numerical blowing up of the computed solutions f or A.

It results from this sensitivity of the solutions to the initial condition that we get a very accurate test to compute a critical initial condition. But we need a good accuracy along the computations ; in our implementation, the numerical tests depend on several relative precisions that we can control. In the last computations, the tests, at each step, for the determination of the steplength, the intermediate values in the Runge-Kutta method, and the two bisection

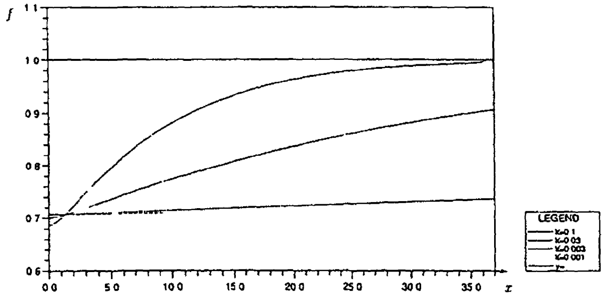

Figure 6. — The computed solutions f of the GL equations when $h = H^c_{sh}$

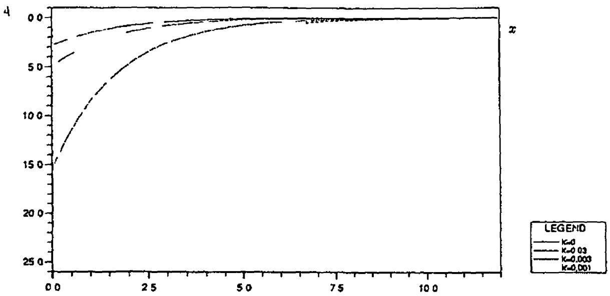

Figure 7. — The computed solutions A of the GL equations when $h = H^c_{sh}$

methods on f_0 and h, are used in general with a 10^{-10}-precision (in double precision) But the tests $A_t > \epsilon_1$ and $C_t < -\epsilon_2$ can be less accurate in order to determine the type of a computed solution Y^{ap}

Remark 4 3 As mentioned above, we control at each step the value of the left hand side of the conservation law (2 25) We observe that, as long as the sequences f_t and A_t slowly vary, the left hand side of (2 25) is of order 10^{-8} This is a very satisfactory result We lose this precision when the numerical blowing up which was just mentioned above appears

Let us now compare our numerical results with the values obtained in Section 2 The following figures give for $\kappa = 0\ 003$, f_0^c and A_0^c as function of h for the GL equations (that is the preceding results) and for the approximate model of Section 2 For this last problem, we use a parametrization by f_0 of the expression $A(0) = -\dfrac{h}{f_0}\tanh(f_0 D)$ (see (2 4)), using the relations (2 29) and (2 31) The intermediate $y = f_0 D$ are given by a Newton method from (2 29)

We verify that the curves are very closed to each other and this justify the use of the approximate model in order to get qualitative results on the problem.

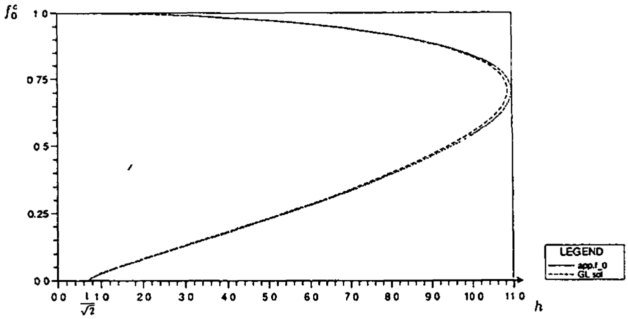

Figure 8. — Comparison of $f_0^c(h)$ for the GL equations and the approximate model when $\kappa = 0.003$.

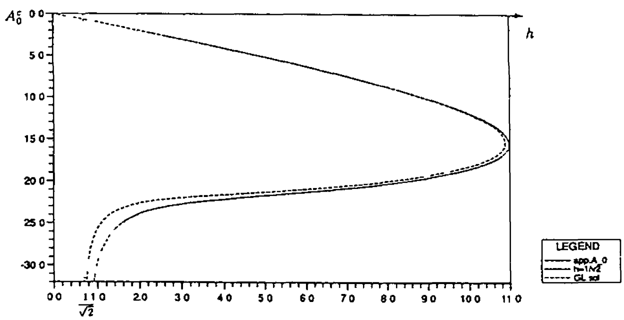

Figure 9. — Comparison of $A_0^c(h)$ for the GL equations and the approximate model when $\kappa = 0.003$.

4.2.3. *Computations of the superheating field*

We get the following critical values for the superheating field :

κ	10^{-3}	3.10^{-3}	10^{-2}	3.10^{-2}	10^{-1}	3.10^{-1}
H_{sh}^c	18.81547	10.8775	5.98527	3.50029	1.99985	1.280063
H_{sh}^c/H_c	26.6091	15.3831	8.46445	4.95015	2.82822	1.81028
δ	0.841454	0.842566	0.84644	0.85739	0.89436	0.99153
$10^2 . \Delta$	$6.6260.10^{-2}$	$1.9859.10^{-1}$	6.5800	1.9617	6.3582	1.7914
Δ/κ	0.6626	0.66197	0.65980	0.654	0.6358	0.5971

where

$$\delta = \kappa^{1/2} H_{sh}^c / H_c \quad \text{and} \quad \Delta = \kappa^{1/2} 2^{3/4} H_{sh}^c - 1 .$$

What appears immediately is that Δ/κ is nearly constant and that this constant becomes very close to the coefficient $15\sqrt{2}/32 \approx 0.6629$ given by Parr in [27] (see Subsection 4.1 where these results are analyzed), as κ tends to 0. If we compare our computed values of δ and Δ/κ with, resp., the constant $2^{-1/4} \approx 0.840896$ in [26] (see (4.1)) and 0.6629 in [27] (see (4.5)), we get :

κ	10^{-3}	3.10^{-3}	10^{-2}	3.10^{-2}	10^{-1}	3.10^{-1}
ϵ_0	$5.6 \cdot 10^{-4}$	$1.7 \cdot 10^{-3}$	$5.5 \cdot 10^{-3}$	$1.6 \cdot 10^{-2}$	$5.3 \cdot 10^{-2}$	0.15
ϵ_1	-3.10^{-4}	-9.10^{-4}	-3.10^{-3}	-9.10^{-3}	-3.10^{-2}	-6.10^{-2}

with

$$\epsilon_0 = \delta - 0.840896 , \quad \epsilon_1 = \Delta/\kappa = - 0.6629 .$$

These results lead us to think that the expansion of $\kappa^{1/2} H_{sh}$, for small κ, can be written with powers of κ ; this is in opposition with the expansion given by the approximate model, in Section 2, which is in powers of $(\kappa \cdot \ln(\kappa))$.

Remark 4.4 : An important error in these computations appears when computing the difference between two very closed quantities for the calculation of Δ. As an example, when $\kappa = 3.10^{-3}$, we get $\Delta = 2^{3/4} \kappa^{1/2} H_{sh}^c - 1 \approx 6.6.10^{-4}$, so that we need five true digits for H_{sh}^c in order to have only one true digit for Δ.

Another interesting value is the initial condition f_0 associated to the superheating field. We get in our computations :

κ	10^{-3}	3.10^{-3}	10^{-2}	3.10^{-2}	10^{-1}	3.10^{-1}
f_0^c	0.70689	0.70646	0.7050	0.7007	0.6874	0.656
β	0.22	0.22	0.21	0.21	0.20	0.17

where :

$$\beta = \frac{2^{-1/2} - f_0}{\kappa} .$$

These numerical results are also in good agreement with the expressions of f_0 given in ([27]). H. Parr gives the following expansion for small κ :

$$f_0(H_{sh}) = \frac{1}{\sqrt{2}} - \frac{7}{32}\kappa \quad \text{with} \quad \frac{7}{32} \approx 0.219 . \tag{4.10}$$

Remark 4.5 : It would be better to have more accuracy on f_0 in order to compute β ; f_0 is very close to $2^{-1/2}$ so that we have the same difficulty as for the calculation of Δ. When $\kappa = 3.10^{-3}$, we need four true digits on f_0 to get only one true digit on $(2^{-1/2} - f_0)$.

All these computations have been performed on the VAX 4000-500 of Ecole Centrale de Nantes. More details on the algorithm are given in [4].

CONCLUSION

When κ is small, our numerical results fit very well with formulas (4.5) and (4.10) given by H. Parr in [27], both for the superheating field and the corresponding value of f_0. Formula (4.5) appears as an improvement of the formula (4.1) given by P. G. de Gennes in [19] and the Orsay group in [26]. On the contrary, these numerical results do not agree with the asymptotic formula that we have obtained in Section 2 by considering an approximate problem. They show that the best we can hope from the approximate model is an approximation of the superheating field modulo $\mathcal{O}(\kappa \ln (\kappa^{-1}))$. But this approximate model is not bad in order to study the qualitative properties of the real problem.

A complete theoretical study of the Ginzburg-Landau equations in $]0, \infty[$ would be of course quite interesting. Some results are given in [8] and [10].

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