NONDIFFERENTIABLE POTENTIALS FOR NONEQUILIBRIUM STEADY STATES

By

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IMA Preprint Series # 284

November 1986

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August 1986

PACS-86 : 05.40.+j , 05.70.Ln

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Abstract

In the weak noise limit of Fokker-Planck models, the stationary probability density can be expressed in the form $P \sim \exp(-1/\epsilon \phi(x))$, where ϵ measures the strength of the noise. We show firstly that, although in general ϕ is not differentiable, it is regular enough to allow its use as a Lyapounov function for the underlying deterministic dynamical system. This justifies the interpretation of ϕ as a generalized thermodynamic potential for systems away from equilibrium.

Secondly, we show that the nondifferentiability of ϕ does not presuppose any kind of irregular behavior in the underlying deterministic system, nor the presence of several stationary points. We construct a simple model with one single attractor and trivial deterministic dynamics, that has a nondifferentiable quasipotential ϕ . We relate the nondifferentiability to the existence of caustics and shock lines in the associated variational problem.

1.1 Introduction

Dynamical systems perturbed by a small random force appear naturally in a variety of physical contexts. An example are Fokker-Planck models of systems away from equilibrium, when considered in the thermodynamical limit. In stationary states the corresponding probability density takes the role of the Gibbs measures in equilibrium.

We consider a system defined by the equations

$$\dot{x}^i(t) = K^i(x) + \sqrt{\epsilon} \sum_j g^i_j(x) \xi^j(t) \quad , \quad i = 1, \dots, n \quad (1.1)$$

where x, K, ξ are in $\mathbb{R}^n$, $g(x)$ is an $n \times n$ matrix and $\dot{x} = dx/dt$. It consists of a deterministic system with a small white noise ξ with mean value and correlation given by

$$\langle \xi^i(t) \rangle = 0 \quad (1.2)$$

$$\langle \xi^i(t_1) \xi^j(t_2) \rangle = \delta(t_1 - t_2) \delta^{ij} \quad (1.3)$$

The parameter ϵ measures the intensity of the noise. Eq. (1.1) is interpreted in the Stratonovich sense. We are interested in the stationary probability density $P(x, \epsilon)$ which is the normalized solution of the Fokker-Planck equation

$$\sum_i \frac{\partial}{\partial x^i} \left[\left[K^i(x) + \epsilon l^i(x) \right] P \right] + \frac{1}{2} \sum_{i,j} \frac{\partial^2}{\partial x^i \partial x^j} \left[\epsilon Q^{ij}(x) P \right] = 0 \quad (1.4)$$

$Q(x)$ is the diffusion tensor (symmetric , positive) , and $l(x)$ is the noise-induced drift (which is irrelevant in the weak noise limit) .

It is known⁽¹⁾ that under quite general conditions, for $\epsilon \rightarrow 0$, P is asymptotically of the form

$$P(x,\epsilon) \sim \exp \left[- \frac{1}{\epsilon} \phi(x) + O(\epsilon^0) \right] \quad (1.5)$$

It is also known⁽¹⁻⁸⁾ , that in general the pseudopotential ϕ is not necessarily differentiable.

The purpose of this article is twofold : We first show that, although the quasipotential ϕ is not differentiable, it is regular enough to be used as a generalized Lyapounov function for the underlying deterministic system. This justifies its interpretation as a thermodynamic potential in nonequilibrium situations. Secondly, we show that nondifferentiable quasipotentials do not presuppose any kind of irregular behavior in the underlying deterministic system, nor the existence of several stationary points (or orbits). We construct a simple example with nondifferentiable ϕ in two dimensions, with a single global attractor. Its behavior is trivial ; all its trajectories are straight lines flowing radially into the attractor. We use tools of the calculus of variations to determine explicitly the points where the corresponding quasipotential is singular.

1.2 Variational representation of φ

The pseudo-potential $\varphi(x)$ is defined variationally by minimalization of an action functional S within the set of absolutely continuous functions⁽¹⁾ $\tilde{x}(t)$:

$$\begin{aligned} S(\tilde{x}(t); x_0, x, T_1, T_2) &= \int_{T_1}^{T_2} dt \quad L(\tilde{x}, \dot{\tilde{x}}) \\ &\equiv \int_{T_1}^{T_2} dt \sum_{i,j} \frac{1}{2} Q^{-1}_{ij} [\dot{\tilde{x}}^i - K^i(\tilde{x})] [\dot{\tilde{x}}^j - K^j(\tilde{x})] \quad (1.6) \end{aligned}$$

If K has a single attractor A , φ is given by

$$\begin{aligned} \varphi(x) = \min_{\substack{\tilde{x}(T_1)=x_0 \in A \\ \tilde{x}(T_2)=x}} [S(\tilde{x}(t); x_0, x)] + c \end{aligned} \quad (1.7)$$

where x_0 lies on the attractor, T_1, T_2 are free and c is a constant. In the case of several stationary points A_i , φ is obtained by calculating for each A_i

$$\begin{aligned} \varphi_i(x) = \min_{\substack{\tilde{x}(T_1)=x_{0i} \in A_i \\ \tilde{x}(T_2)=x}} [S(\tilde{x}(t); x_{0i}, x)] + c_i \end{aligned} \quad (1.8)$$

and then taking the minimum over the A_i 's

$$\varphi(x) = \min_i \varphi_i(x) + c' \quad (1.9)$$

The weighting constants c_i are determined by methods of Markov chains⁽¹⁾.

The Hamiltonian associated by Legendre transformation to the Lagrangian L of Eq. (1.6) is

$$H = \frac{1}{2} \sum_{i,j} Q^{ij} p_i p_j + \sum_i p_i K^i \quad (1.10)$$

$$\text{where } p_i = \frac{\partial L}{\partial \dot{x}_i} = \sum_j Q_{ij}^{-1} [\dot{\tilde{x}}^j - K^j(\tilde{x})] \quad (1.11)$$

At the points where φ is differentiable p_i is equal to

$$p^i = \frac{\partial \varphi}{\partial x^i} \quad (1.12)$$

The minimalization of $S(\tilde{x}(t); x_0, x, T_1, T_2)$ with variable initial and final times T_1, T_2 is equivalent to the minimalization of S with fixed $T_1 = -\infty$ and $T_2 = 0$.^(1,2) The condition for the parametrization of time in $\tilde{x}(t)$ to minimize S among all possible parametrizations leads to the constraint^(1,2)

$$H(x,p) = 0 \quad (1.13)$$

We have thus a classical variational problem with a constraint of zero energy.

Although in general $\bar{\varphi}_i(x)$ and $\varphi(x)$ are not necessarily differentiable, they cannot be arbitrarily irregular either : it can be proven⁽¹⁾ that they satisfy a local Lipschitz condition, which implies almost everywhere differentiability⁽⁹⁾. We will show that this property is enough to allow the use of the quasipotential φ as a generalized Lyapounov function for the deterministic system.

2. Quasipotential as nondifferentiable Lyapounov function

Models representing thermodynamic equilibrium satisfy the conditions of detailed balance, which imply differentiability of the quasipotential^(3,7). In this case φ can be identified with the negative of the thermodynamic entropy (through the Boltzmann relation $\mathcal{S} = k_B \ln P$, taking $\epsilon = k_B$). Its main characteristic is that φ is a Lyapounov function for the underlying deterministic equation

$$\dot{x}^i = K^i(x) \quad (2.1)$$

$\varphi(x(t))$ decreases monotonically along the trajectories of (2.1) :

$$\frac{d\varphi}{dt} = \sum_i \frac{\partial \varphi}{\partial x^i} \dot{x}^i = \sum_i \frac{\partial \varphi}{\partial x^i} K^i = - \sum_{i,j} Q^{ij} p_i p_j < 0 \quad (2.2)$$

for $p > 0$. Here we have used Eqs. (2.1), (1.13), (1.14) and the fact that Q is positive definite.

In nonequilibrium situations the quasipotential has been proposed as a natural generalization of the thermodynamic potentials. ⁽³⁻⁵⁾ For this generalization to be meaningful it is necessary that φ decreases along the trajectories. Although the argument of Eq. (2.2) cannot be applied where φ is not differentiable, we will show that the Lipschitz condition is enough to guarantee this behavior.

The theory of nondifferentiable Lyapounov functions was developed by T. Yoshizawa^(10,11). The main result is that, provided that φ is Lipschitz and it decreases along the trajectories, all the theorems for the differentiable case can be generalized.

We know from Eqs. (1.10), (1.12), and (1.13) that wherever φ is differentiable it satisfies $\sum K^i \partial\varphi/\partial x^i < 0$. We need thus to prove that the validity of this condition almost everywhere in R^n implies the decrease of φ along all trajectories. We distinguish two situations :

a) Consider a segment of a trajectory, such that its points at which φ is nondifferentiable are of measure zero with respect to the (one dimensional) restriction of the Lebesgue measure on the trajectory. Then the difference in φ between two points of the trajectory is given by

$$\varphi(x(t_2)) - \varphi(x(t_1)) = \int_{t_1}^{t_2} dt \left\{ \frac{d\varphi(x(t))}{dt} \right\} = \int_{t_1}^{t_2} dt \left\{ \sum_i \frac{\partial\varphi}{\partial x^i} K^i \right\} < 0 \quad (2.3)$$

where $x(t_1)$ and $x(t_2)$ are two points of the segment such that $t_2 > t_1$. The

curly brackets indicate that the functions appearing under the integral only need to be defined almost everywhere (with respect to the restricted measure).

b) The other possibility is that, on a segment of the trajectory, the set of points at which φ is nondifferentiable is of positive measure with respect to the restricted measure. In this case, since φ is almost everywhere differentiable in R^n , there exists a smooth curve $\Gamma : x = \gamma(t)$, parametrized by $t_1 \leq t \leq t_2$ that satisfies the following properties :

- i) $\gamma(t_1) = x(t_1)$ and $\gamma(t_2) = x(t_2)$
- ii) $\gamma(t)$ and $d\gamma(t)/dt$ are as close to $x(t)$ and $dx(t)/dt$ as wanted, (as defined e.g. by the distance $\sup_{\{t\}} \{ |x(t) - \gamma(t)| + |\dot{x}(t) - \dot{\gamma}(t)| \}$).
- iii) on the curve Γ , φ is almost everywhere differentiable with respect to the restriction of Lebesgue measure on it.

The continuity of φ implies that

$$\varphi(x(t_2)) - \varphi(x(t_1)) = \int_{t_1}^{t_2} dt \left\{ \sum_i \frac{\partial \varphi(\gamma)}{\partial \gamma^i} \dot{\gamma}^i(t) \right\} \quad (2.4)$$

and the property ii) implies that this expression is as close as wanted to

$$\int_{t_1}^{t_2} dt \left\{ \sum_i \frac{\partial \varphi(\gamma)}{\partial \gamma^i} K^i(\gamma(t)) \right\} < 0 \quad (2.5)$$

which implies the decrease of φ along the trajectory $x(t)$.

Thus φ decreases along all trajectories; this property allows the interpretation of φ as a thermodynamic potential.

3. Simple model with nondifferentiable quasipotential

3.1 Definition of the model

In this section we construct a very simple model in two dimensions, of a general type first proposed in Ref. (2), that displays a nondifferentiable quasipotential. We calculate φ and localize its singularities explicitly.

We define the model in polar coordinates. The radial and angular components of the drift are given by

$$\begin{aligned} K^r(r, \theta) &= -r (1 + \alpha f(r) g(\theta)) \\ K^\theta(r, \theta) &= 0 \end{aligned} \quad (3.1)$$

The functions f and g are defined as

$$\begin{aligned} f(r) &= h(r; r_1, r_2) \\ g(\theta) &= h(\theta; \theta_1, \theta_2) \end{aligned} \quad (3.2)$$

where

$$h(z; z_1, z_2) = \begin{cases} 1 + a_2 (z-z_0)^2 + a_4 (z-z_0)^4 + a_6 (z-z_0)^6, & \text{if } z_1 \leq z \leq z_2 \\ 0 & , \text{otherwise} \end{cases} \quad (3.3)$$

The coefficients are chosen such that h vanishes together with its first and second derivatives at the points z_1 and z_2 , and is equal to 1 in the middle of the interval $z_0 = (z_1 + z_2)/2$, (see Fig. 1). We have chosen the

boundaries $r_1=0.3$, $r_2=0.9$, $\theta_1= 30^0$, $\theta_2= -30^0$. We chose $\alpha=2$ so that the effect of the perturbation is easily visible. The drift K is thus twice continuously differentiable. It is linear everywhere except inside of the annular disk (A) shown in Fig. 2 and defined by $r_1 \leq r \leq r_2$ and $\theta_1 \leq \theta \leq \theta_2$. There the radial component is more strongly attractive towards the origin. K is symmetric with respect to the x -axis.

The trajectories of the corresponding deterministic system (2.1) are all straight lines going radially into the single attractor located at the origin. When a trajectory goes through the region A the only modification produced by the perturbation is that the radial velocity towards the attractor is increased.

We calculate the quasipotential ψ by solving numerically the characteristic equations of the associated Hamiltonian system. They are given by

$$\begin{aligned} \dot{r} &= \frac{\partial H}{\partial p_r} = p_r + K^r \\ \dot{p}_r &= - \frac{\partial H}{\partial r} = -p_r \frac{\partial K^r}{\partial r} \\ \dot{\theta} &= \frac{\partial H}{\partial p_\theta} = p_\theta \\ \dot{p}_\theta &= - \frac{\partial H}{\partial \theta} = -p_r \frac{\partial K^r}{\partial \theta} \\ \dot{\psi} &= \frac{\partial \psi}{\partial r} (p_r + K^r) + \frac{\partial \psi}{\partial \theta} p_\theta \end{aligned} \tag{3.4}$$

The solutions must satisfy the constraints

$$\begin{aligned} & H(x,p)=0 \\ \text{and} \quad & x(t \rightarrow -\infty) = 0. \end{aligned} \quad (3.5)$$

The quasipotential ϕ is obtained by minimalization of ψ as explained below. In the unperturbed region outside A, the solution satisfying these constraints is given by

$$\begin{aligned} r(t) &= r_0 \exp(t) & , & & p_r(t) &= 2 r_0 \exp(t) \\ \theta(t) &= \theta_0 & , & & p_\theta(t) &= 0 \\ \psi(t) &= r^2(t) = r_0^2 \exp(2t) \end{aligned} \quad (3.6)$$

Since in the numerical computation one cannot start with the initial conditions at the critical point, we take the initial conditions on a circle C of radius $r_0=0.2$ and center at the origin. We set there the time origin $t=0$. Since this circle is outside the region A, the values of the initial conditions are determined by Eq. (3.6). Through each point (r_0, θ_0) on the circle C passes a single trajectory. The initial values for the rest of the variables is determined by the relations

$$\begin{aligned} p_r(r_0, \theta_0) &= 2 r_0 \\ p_\theta(r_0, \theta_0) &= 0 \\ \psi(r_0, \theta_0) &= r_0^2 \end{aligned} \quad (3.7)$$

The solutions $r(t)$, $\theta(t)$ are extremals of the variational problem defined by the action (1.6). In a region close to the initial point they are locally minimizing solutions. But at some point the trajectories can cease to be local minimizers. It is known, that the value of ψ at any point of the plane is given by the value of ψ as obtained along one smooth locally minimizing solution $(r(t), \theta(t))$ of the above equations⁽²⁾. However, it is possible that there are several locally minimizing trajectories going through a given point x . Each of them can give a different value of ψ . Following Eq. (1.7), ϕ at that point is equal to the global minimum among the $\psi(x)$'s .

Thus, in order to determine ϕ we proceed in two steps :

1) Starting at points on the circle C , we calculate the extremal trajectory (using a Runge-Kutta algorithm). At each point on the trajectory we check if the extremal is still a local minimizer, by means of the criteria developed among others by Jacobi and Kneser.⁽¹²⁻¹⁴⁾ After the first point at which it ceases to be a local minimum, the rest of the trajectory can be discarded.

2) Then at each point, the global maximum is identified among the local ones. For our simple model this can be done relatively easily, but for general problems it can be a difficult problem.

A feature that makes things simple in our model is the symmetry with respect to the x -axis : If a local minimizer starting at (r_0, θ_0) reaches the x -axis, it will meet there another local minimizer with initial point

$(r_0, -\theta_0)$. As we will see, ψ grows monotonically along the extremals. Thus, a local minimizer cannot be a global minimizer after it crosses the x-axis. We therefore only need to consider the trajectories until the first point where such a crossing occurs.

The property of growth of ψ along the extremals follows immediately from Eqs. (3.4), (1.12) and the constraint

$$0 = H = \frac{1}{2} p_r^2 + p_r K^r + \frac{1}{2} p_\theta^2 \quad (3.8)$$

which implies $p_r K^r \geq 0$. Together with Eqs. (3.4) and (1.12) it gives

$$\frac{d\psi}{dt} = p_r \dot{r} + p_\theta \dot{\theta} = p_r^2 + p_r K^r + p_\theta^2 \geq 0 \quad (3.9)$$

3.2 Local minimizers

A detailed presentation of the methods used in this section can be found in References (12-14).

Since the criteria for an extremal to be a local minimum cannot be applied directly to the case in which the extremals start at a critical point, we reformulate the problem as a variational problem with fixed endpoint and variable initial point lying on a curve: For a fixed endpoint P_2 , the set of locally minimalizing trajectories with initial point at the critical point, coincides with the set of trajectories that locally minimize S among all curves with initial point on the circle C and endpoint P_2 .

From the four necessary and sufficient conditions for a segment of an extremal to be a minimizer (Legendre condition, Weierstrass condition, transversality and Jacobi condition), the first two are satisfied identically in the present model. The transversality condition determines the angle at which the minimizer crosses the initial curve C. For a curve parametrized by $\mu : r = \beta^1(\mu), \theta = \beta^2(\mu)$, the transversality condition can be stated (using the Lagrangian $L(r, \dot{r}, \theta, \dot{\theta})$) as

$$\frac{\partial L}{\partial \dot{r}} \frac{\partial \beta^1}{\partial \mu} + \frac{\partial L}{\partial \dot{\theta}} \frac{\partial \beta^2}{\partial \mu} = 0 \quad (3.10)$$

For the circle C, parametrized by the initial angle θ_0 , this gives

$$\frac{\partial L}{\partial \dot{\theta}} = p_{\theta}(r_0, \theta_0) = 0 \quad (3.11)$$

This condition is automatically satisfied due to the constraints (3.5), (see Eq. (3.7)).

Thus the criterion of minimality in the present situation depends only on the Jacobi condition, which can be formulated as follows : The set of trajectories that we consider is a one-parameter family of extremals, that may have an envelope. (An example of this phenomenon is the caustics found in optics). The criterion states that a given extremal ceases to be a local minimum at its first point of contact with the envelope of the family. The location of the envelope can be determined as follows : If we denote by $z^1(t, \theta_0) \equiv r(t, \theta_0)$, $z^2(t, \theta_0) \equiv \theta(t, \theta_0)$ the family of extremals

parametrized by θ_0 , and we define the functions u^1 and u^2 as

$$u^i(t, \theta_0) \equiv \frac{\partial z^i}{\partial \theta_0}, \quad i=1,2. \quad (3.12)$$

then the envelope will consist of the points at which the following determinant becomes zero

$$\Delta(z^1(t, \theta_0), z^2(t, \theta_0)) \equiv \frac{\partial z^1}{\partial t} \frac{\partial z^2}{\partial \theta_0} - \frac{\partial z^2}{\partial t} \frac{\partial z^1}{\partial \theta_0} \quad (3.13)$$

The functions u^1, u^2 satisfy, for fixed θ_0 , the Jacoby equations

$$\frac{d}{dt} \left[\sum_i \left(\frac{\partial^2 L}{\partial \dot{z}^k \partial z^i} u^i + \frac{\partial^2 L}{\partial \dot{z}^k \partial \dot{z}^i} \dot{u}^i \right) \right] = \sum_i \left(\frac{\partial^2 L}{\partial z^k \partial z^i} u^i + \frac{\partial^2 L}{\partial z^k \partial \dot{z}^i} \dot{u}^i \right) \quad (3.14)$$

where $k=1,2$. They are a system of two second order linear differential equations, in which the t -dependent coefficients are evaluated along the considered extremal. The initial conditions for u^1 and u^2 on the circle C can be calculated from Eqs. (3.6) and (3.12) :

$$\begin{aligned} u^1(t=0, \theta_0) &= 0, & \dot{u}^1(t=0, \theta_0) &= 0 \\ u^2(t=0, \theta_0) &= 1, & \dot{u}^2(t=0, \theta_0) &= 0 \end{aligned} \quad (3.15)$$

Thus, by solving numerically the system of equations consisting of Eqs. (3.4) and (3.14), and calculating at each point the determinant (3.13), we can determine on each extremal the point at which it ceases to be a local minimum.

3.3 Results

Figure 2a shows the behavior of the one parameter family of extremals that go through the perturbed region A. As we have mentioned earlier we only need to consider the extremals until the points where they cross the x-axis. The extremals can be divided into four subsets that have qualitatively different behavior: (a) if $30^0 < |\theta_0| < 180^0$, (b) if $26.5^0 < |\theta_0| \leq 30^0$, (c) if $19.5^0 < |\theta_0| < 26.5^0$, (d) If $|\theta_0| < 19.5^0$.

The extremals belonging to the subset (a) do not enter the perturbed region A and thus are radial straight lines. The extremals belonging to (b) enter the region A and are bent, but they do not form an envelope. All points that are reached by extremals of (a) or (b) before they cross the x-axis are not reached by any other minimizer. Thus ψ is determined by the corresponding single value of ψ .

The extremals of the subsets (c) and (d) with positive θ_0 have an envelope with two branches separated by a cusp. The subsets (c) and (d) generate the left and right branches respectively. The same applies for negative θ_0 's. The location of the envelopes can be seen in Fig. 2a and in more detail in Fig. 2b, which a magnification of the region close to the envelope. The trajectories are drawn only until the point where they touch the envelope. The right branches of the envelope (generated by (d)) each lie completely on one side of the x-axis, whereas the left branches (generated by (c)) cross the x-axis. In the figures they are only drawn up to the point at which this crossing occurs. In the region located between the two

branches of the envelope, each point is reached by two locally minimalizing extremals. One belongs to the subset (c) and the other to the subset (d). At each of these points, ϕ is determined by the minimum of the two corresponding ψ 's.

Figure 3 shows a representation of $\phi(r,\theta)$ in terms level curves, calculated by the procedure described above. In the region between the two branches of the envelope, the two solid lines represent the points at which the two values of ψ are equal. However, the values of $(p_r, p_\theta) = (\partial\psi/\partial r, \partial\psi/\partial\theta)$ at these points, when calculated along different minimizers are not the same. Therefore ϕ is not differentiable on this two lines.

The minimizers of the subset (b) cross each other pairwise on a half line contained in the x-axis. On this half line, also marked by a solid line in Fig. 3, ϕ is also not differentiable by the same argument as above.

3.4 Conclusion

The set of points at which ϕ is not differentiable consists thus of a half line, contained in the x-axis, and two lateral segments, located in the region between the two branches of the envelope. This set of the points at which two local minimizers cross, having the same values of ψ but different values of (p_r, p_θ) . In this context the lines where ϕ is not differentiable are called shock lines.

For the example shown in Figs. 2 and 3 we have chosen a relatively large perturbation ($\alpha = 2$ in Eq. (3.1)) to facilitate the graphical display. If α is taken smaller, the picture stays qualitatively the same. The location of the envelope and of the shock line is displaced to the right, and the two side segments become shorter. The possibility that for small enough α the side segments degenerate into a point cannot be excluded, but we have not observed it.

Although the present model is very simple, it displays the basic mechanism that produces nondifferentiability of ϕ in more complex models. We notice that the same construction that we have made, involving a local perturbation of a linear system, can be applied to systems in which the unperturbed drift is a gradient field with one single attractor. Such models will display behavior that is qualitatively similar to the present one.

We notice that although it is very easy to determine numerically the local minimizers, there is no simple systematic method to choose at each point the global minimum among them.

Acknowledgements

I would like to thank Martin Day and Mete Soner for very helpful discussions. I also would like to thank the Institute for Mathematics and its Applications at the University of Minnesota for its friendly hospitality during the 1985-86 academic year. This work has been partially supported by the Swiss National Science Foundation (Grant No. 82.278.0.85).

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Figure captions

Fig. 1 : Graph of the function $h(z; z_1, z_2)$

Fig. 2 : a) Behavior of the extremals in the perturbed region A (delimited by a broken line). The extremals are drawn only up to the points at which they cross the x-axis or reach the envelope and cease to be local minima.

b) Magnification of a) showing in more detail the envelope (dotted line) and the crossings of the two subsets of local minimizers.

Fig. 3 : a) Level curves of the quasipotential ϕ . The spacing of the levels is chosen in such a way that, in absence of the perturbation the distance between successive curves would be uniform ($\sim r^2$). The solid line represents the points at which ϕ is not differentiable.

b) Magnification of a) showing in more detail the level curves in the region close to the envelope (dotted line) and the determination of the location of the shock line (solid line).

Figure 1

Figure 2a

Figure 2b

Figure 3a

Figure 3b

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