Preface

This textbook is intended for use by students of physics, physical chemistry, and theoretical chemistry. The reader is presumed to have a basic knowledge of atomic and quantum physics at the level provided, for example, by the first few chapters in our book *The Physics of Atoms and Quanta*. The student of physics will find here material which should be included in the basic education of every physicist. This book should furthermore allow students to acquire an appreciation of the breadth and variety within the field of molecular physics and its future as a fascinating area of research.

June 2016

Walter Olthoff
Program Chair
ECOOP 2016

Organization

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Part I

Hamiltonian Mechanics

Hamiltonian Mechanics unter besonderer Berücksichtigung der höhereren Lehranstalten

Ivar Ekeland[1], Roger Temam[2] Jeffrey Dean, David Grove, Craig Chambers, Kim B. Bruce, and Elsa Bertino

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F-91405 Orsay Cedex, France

Abstract. Özet yazısı ...

Keywords: computational geometry, graph theory, Hamilton cycles

1 Fixed-Period Problems: The Sublinear Case

With this chapter, the preliminaries are over, and we begin the search for periodic solutions to Hamiltonian systems. All this will be done in the convex case; that is, we shall study the boundary-value problem

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with $H(t,\cdot)$ a convex function of x, going to $+\infty$ when $\|x\| \to \infty$.

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In this section, we will consider the case when the Hamiltonian $H(x)$ is autonomous. For the sake of simplicity, we shall also assume that it is C^1.

We shall first consider the question of nontriviality, within the general framework of (A_∞, B_∞)-subquadratic Hamiltonians. In the second subsection, we shall look into the special case when H is $(0, b_\infty)$-subquadratic, and we shall try to derive additional information.

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Proof. Condition (7) means that, for every $\delta' > \delta$, there is some $\varepsilon > 0$ such that

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It is an exercise in convex analysis, into which we shall not go, to show that this implies that there is an $\eta > 0$ such that

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Corollary 1. *Assume H is C^2 and (a_∞, b_∞)-subquadratic at infinity. Let $\xi_1, \ldots, \xi_N$ be the equilibria, that is, the solutions of $H'(\xi) = 0$. Denote by ω_k the smallest eigenvalue of $H''(\xi_k)$, and set:*

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But this index is precisely the index $i_T(\widetilde{x})$ of the T-periodic solution $\widetilde{x}$ over the interval $(0,T)$, as defined in Sect. 2.6. So

$$i_T(\widetilde{x}) = 0 \ . \tag{21}$$

Now if $\widetilde{x}$ has a lower period, T/k say, we would have, by Corollary 31:

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This would contradict (21), and thus cannot happen. □

Notes and Comments. The results in this section are a refined version of [1]; the minimality result of Proposition 14 was the first of its kind.

To understand the nontriviality conditions, such as the one in formula (16), one may think of a one-parameter family x_T, $T \in \left(2\pi\omega^{-1}, 2\pi b_\infty^{-1}\right)$ of periodic solutions, $x_T(0) = x_T(T)$, with x_T going away to infinity when $T \to 2\pi\omega^{-1}$, which is the period of the linearized system at 0.

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Assume also that H is C^2, and $H''(t,x)$ is positive definite everywhere. Then there is a sequence x_k, $k \in \mathbb{N}$, of kT-periodic solutions of the system

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$\square$

*Example 1 (*External forcing*).* Consider the system:

$$\dot{x} = JH'(x) + f(t) \tag{29}$$

where the Hamiltonian H is $(0, b_\infty)$-subquadratic, and the forcing term is a distribution on the circle:

$$f = \frac{d}{dt} F + f_o \qquad \text{with} \quad F \in L^2 \left(\mathbb{R}/T\mathbb{Z}; \mathbb{R}^{2n} \right) \ , \tag{30}$$

where $f_o := T^{-1} \int_o^T f(t) dt$. For instance,

$$f(t) = \sum_{k \in \mathbb{N}} \delta_k \xi \ , \tag{31}$$

where δ_k is the Dirac mass at $t = k$ and $\xi \in \mathbb{R}^{2n}$ is a constant, fits the prescription. This means that the system $\dot{x} = JH'(x)$ is being excited by a series of identical shocks at interval T.

Definition 1. *Let $A_\infty(t)$ and $B_\infty(t)$ be symmetric operators in $\mathbb{R}^{2n}$, depending continuously on $t \in [0,T]$, such that $A_\infty(t) \leq B_\infty(t)$ for all t.*

A Borelian function $H : [0,T] \times \mathbb{R}^{2n} \to \mathbb{R}$ is called (A_∞, B_∞)-subquadratic at infinity if there exists a function $N(t,x)$ such that:

$$H(t,x) = \frac{1}{2} \left(A_\infty(t) x, x \right) + N(t,x) \tag{32}$$

$$\forall t \ , \quad N(t,x) \qquad \text{is convex with respect to} \quad x \tag{33}$$

$$N(t,x) \geq n \left(\|x\| \right) \qquad \text{with} \quad n(s) s^{-1} \to +\infty \quad \text{as} \quad s \to +\infty \tag{34}$$

$$\exists c \in \mathbb{R} \ : \quad H(t,x) \leq \frac{1}{2} \left(B_\infty(t) x, x \right) + c \quad \forall x \ . \tag{35}$$

If $A_\infty(t) = a_\infty I$ and $B_\infty(t) = b_\infty I$, with $a_\infty \leq b_\infty \in \mathbb{R}$, we shall say that H is (a_∞, b_∞)-subquadratic at infinity. As an example, the function $\|x\|^\alpha$, with $1 \leq \alpha < 2$, is $(0, \varepsilon)$-subquadratic at infinity for every $\varepsilon > 0$. Similarly, the Hamiltonian

$$H(t,x) = \frac{1}{2} k \|k\|^2 + \|x\|^\alpha \tag{36}$$

is $(k, k + \varepsilon)$-subquadratic for every $\varepsilon > 0$. Note that, if $k < 0$, it is not convex.

Notes and Comments. The first results on subharmonics were obtained by Rabinowitz in [5], who showed the existence of infinitely many subharmonics both in the subquadratic and superquadratic case, with suitable growth conditions on H'. Again the duality approach enabled Clarke and Ekeland in [2] to treat the same problem in the convex-subquadratic case, with growth conditions on H only.

Recently, Michalek and Tarantello (see [3] and [4]) have obtained lower bound on the number of subharmonics of period kT, based on symmetry considerations and on pinching estimates, as in Sect. 5.2 of this article.

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Part II

Theoretical Contributions

Hamiltonian Mechanics2

Ivar Ekeland[1] and Roger Temam[2]

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[2] Université de Paris-Sud, Laboratoire d'Analyse Numérique, Bâtiment 425, F-91405 Orsay Cedex, France

Abstract. The abstract should summarize the contents of the paper using at least 70 and at most 150 words. It will be set in 9-point font size and be inset 1.0 cm from the right and left margins. There will be two blank lines before and after the Abstract. ...

Keywords: graph transformations, convex geometry, lattice computations, convex polygons, triangulations, discrete geometry

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$$\dot{x} = JH'(x) + f(t) \tag{29}$$

where the Hamiltonian H is $(0, b_\infty)$-subquadratic, and the forcing term is a distribution on the circle:

$$f = \frac{d}{dt} F + f_o \qquad \text{with} \ \ F \in L^2 \left(\mathbb{R}/T\mathbb{Z}; \mathbb{R}^{2n} \right) \ , \tag{30}$$

where $f_o := T^{-1} \int_o^T f(t) dt$. For instance,

$$f(t) = \sum_{k \in \mathbb{N}} \delta_k \xi \ , \tag{31}$$

where δ_k is the Dirac mass at $t = k$ and $\xi \in \mathbb{R}^{2n}$ is a constant, fits the prescription. This means that the system $\dot{x} = JH'(x)$ is being excited by a series of identical shocks at interval T.

Definition 1. *Let $A_\infty(t)$ and $B_\infty(t)$ be symmetric operators in $\mathbb{R}^{2n}$, depending continuously on $t \in [0,T]$, such that $A_\infty(t) \le B_\infty(t)$ for all t.*

A Borelian function $H : [0,T] \times \mathbb{R}^{2n} \to \mathbb{R}$ is called (A_∞, B_∞)-subquadratic at infinity if there exists a function $N(t,x)$ such that:

$$H(t,x) = \frac{1}{2} \left(A_\infty(t) x, x \right) + N(t,x) \tag{32}$$

$$\forall t \ , \quad N(t,x) \qquad \text{is convex with respect to} \ \ x \tag{33}$$

$$N(t,x) \ge n \left(\|x\| \right) \qquad \text{with} \ \ n(s) s^{-1} \to +\infty \ \ \text{as} \ \ s \to +\infty \tag{34}$$

$$\exists c \in \mathbb{R} \ : \quad H(t,x) \le \frac{1}{2} \left(B_\infty(t) x, x \right) + c \quad \forall x \ . \tag{35}$$

If $A_\infty(t) = a_\infty I$ and $B_\infty(t) = b_\infty I$, with $a_\infty \le b_\infty \in \mathbb{R}$, we shall say that H is (a_∞, b_∞)-subquadratic at infinity. As an example, the function $\|x\|^\alpha$, with $1 \le \alpha < 2$, is $(0, \varepsilon)$-subquadratic at infinity for every $\varepsilon > 0$. Similarly, the Hamiltonian

$$H(t,x) = \frac{1}{2} k \|k\|^2 + \|x\|^\alpha \tag{36}$$

is $(k, k + \varepsilon)$-subquadratic for every $\varepsilon > 0$. Note that, if $k < 0$, it is not convex.

Notes and Comments. The first results on subharmonics were obtained by Rabinowitz in 1988, who showed the existence of infinitely many subharmonics both in the subquadratic and superquadratic case, with suitable growth conditions on H'. Again the duality approach enabled Clarke and Ekeland in 1978 to treat the same problem in the convex-subquadratic case, with growth conditions on H only.

Recently, Michalek and Tarantello (see Michalek, R., Tarantello, G. 1988 and Tarantello, G. (to appear)) have obtained lower bound on the number of subharmonics of period kT, based on symmetry considerations and on pinching estimates, as in Sect. 5.2 of this article.

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