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.

For the student of chemistry, the concepts introduced in this book will provide a theoretical framework for that entire field of study. With the help of these concepts, it is at least in principle possible to reduce the enormous body of empirical chemical knowledge to a few basic principles: those of quantum mechanics. In addition, modern physical methods whose fundamentals are introduced here are becoming increasingly important in chemistry and now represent indispensable tools for the chemist. As examples, we might mention the structural analysis of complex organic compounds, spectroscopic investigation of very rapid reaction processes or, as a practical application, the remote detection of pollutants in the air.

April 1995

Walter Olthoff
Program Chair
ECOOP'95

Organization

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Hamiltonian Mechanics unter besonderer Berücksichtigung der höhreren Lehranstalten

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

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Keywords: computational geometry, graph theory, Hamilton cycles

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

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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

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

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To understand the nontriviality conditions, such as the one in formula (**??**), 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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$$H(t,x) \geq n\left(\|x\|\right) \qquad \text{with} \quad n(s)s^{-1} \to \infty \quad \text{as} \quad s \to \infty \tag{25}$$

$$\forall \varepsilon > 0 \ , \quad \exists c \ : \ H(t,x) \leq \frac{\varepsilon}{2} \left\| x \right\|^2 + c \ . \tag{26}$$

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

$$\dot{x} = JH'(t,x) \tag{27}$$

such that, for every $k \in \mathbb{N}$, there is some $p_o \in \mathbb{N}$ with:

$$p \geq p_o \Rightarrow x_{pk} \neq x_k \ . \tag{28}$$

□

*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:

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

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:

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

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

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

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

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 $\left\| x \right\|^\alpha$, with $1 \leq \alpha < 2$, is $(0, \varepsilon)$-subquadratic at infinity for every $\varepsilon > 0$. Similarly, the Hamiltonian

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

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 [**?**], 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 [**?**] to treat the same problem in the convex-subquadratic case, with growth conditions on H only.

Recently, Michalek and Tarantello (see [**?**] and [**?**]) 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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Hamiltonian Mechanics2

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$$\forall \varepsilon > 0 \ , \quad \exists c \ : \ H(t,x) \le \frac{\varepsilon}{2} \left\|x\right\|^2 + c \ . \tag{26}$$

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

$$\dot{x} = JH'(t,x) \tag{27}$$

such that, for every $k \in \mathbb{N}$, there is some $p_o \in \mathbb{N}$ with:

$$p \ge p_o \Rightarrow x_{pk} \ne x_k \ . \tag{28}$$

$\square$

*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:

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

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:

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

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

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

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

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 $\left\|x\right\|^\alpha$, with $1 \le \alpha < 2$, is $(0, \varepsilon)$-subquadratic at infinity for every $\varepsilon > 0$. Similarly, the Hamiltonian

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

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 **?**, 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 **?** 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. **?** and Tarantello, G. **?**) 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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