## **Preface**

这是一个试验这是一个试验这是一个试验这是一个试验这是一个 试验 试验

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

ECOOP'95 is organized by the department of Computer Science, University of Århus and AITO (association Internationa pour lesTechnologie Object) in cooperation with ACM/SIGPLAN.

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# Table of Contents

## **Hamiltonian Mechanics**

Hamiltonian Mechanics unter besonderer Berücksichtigung der höhreren	
Lehranstalten	1
Ivar Ekeland (Université de Paris-Sud), Jeffrey Dean, David Grove,	
Craig Chambers (Università di Geova), Kim B. Bruce (Stanford Uni-	
versity), Elisa Bertino (Digita Research Center)	
Hamiltonian Mechanics2	7
Author Index	14
Subject Index	14

## Hamiltonian Mechanics unter besonderer Berücksichtigung der höhreren Lehranstalten

Ivar Ekeland<sup>1</sup>, Roger Temam<sup>2</sup> Jeffrey Dean, David Grove, Craig Chambers, Kim B. Bruce, and Elsa Bertino

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WWW home page: http://users/~iekeland/web/welcome.html  $^2$  Université de Paris-Sud, Laboratoire d'Analyse Numérique, Bâtiment 425, F-91405 Orsay Cedex, France

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#### 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

$$\dot{x} = JH'(t, x)$$
$$x(0) = x(T)$$

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

#### 1.1 Autonomous Systems

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  $(A_{\infty}, B_{\infty})$ -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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Theorem 1 tells us that if  $\lambda + \gamma < 0$ , the boundary-value problem:

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has at least one solution  $\overline{x}$ , which is found by minimizing the dual action functional:

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on the range of  $\Lambda$ , which is a subspace  $R(\Lambda)_L^2$  with finite codimension. Here

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is a convex function, and

$$N(x) \le \frac{1}{2} \left( \left( B_{\infty} - A_{\infty} \right) x, x \right) + c \quad \forall x . \tag{6}$$

**Proposition 1.** Assume H'(0) = 0 and H(0) = 0. Set:

$$\delta := \liminf_{x \to 0} 2N(x) \|x\|^{-2} . \tag{7}$$

If  $\gamma < -\lambda < \delta$ , the solution  $\overline{u}$  is non-zero:

$$\overline{x}(t) \neq 0 \quad \forall t \ .$$
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*Proof.* Condition (7) means that, for every  $\delta' > \delta$ , there is some  $\varepsilon > 0$  such that

$$||x|| \le \varepsilon \Rightarrow N(x) \le \frac{\delta'}{2} ||x||^2$$
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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

$$f \|x\| \le \eta \Rightarrow N^*(y) \le \frac{1}{2\delta'} \|y\|^2 . \tag{10}$$

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Since  $u_1$  is a smooth function, we will have  $||hu_1||_{\infty} \leq \eta$  for h small enough, and inequality (10) will hold, yielding thereby:

$$\psi(hu_1) \le \frac{h^2}{2} \frac{1}{\lambda} \|u_1\|_2^2 + \frac{h^2}{2} \frac{1}{\delta'} \|u_1\|^2 . \tag{11}$$

If we choose  $\delta'$  close enough to  $\delta$ , the quantity  $\left(\frac{1}{\lambda} + \frac{1}{\delta'}\right)$  will be negative, and we end up with

$$\psi(hu_1) < 0 \quad \text{for } h \neq 0 \text{ small }.$$
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On the other hand, we check directly that  $\psi(0) = 0$ . This shows that 0 cannot be a minimizer of  $\psi$ , not even a local one. So  $\overline{u} \neq 0$  and  $\overline{u} \neq \Lambda_o^{-1}(0) = 0$ .

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

$$\omega := \operatorname{Min} \left\{ \omega_1, \dots, \omega_k \right\} . \tag{13}$$

*If:* 

$$\frac{T}{2\pi}b_{\infty} < -E\left[-\frac{T}{2\pi}a_{\infty}\right] < \frac{T}{2\pi}\omega\tag{14}$$

then minimization of  $\psi$  yields a non-constant T-periodic solution  $\overline{x}$ .

We recall once more that by the integer part  $E[\alpha]$  of  $\alpha \in \mathbb{R}$ , we mean the  $a \in \mathbb{Z}$  such that  $a < \alpha \le a+1$ . For instance, if we take  $a_{\infty} = 0$ , Corollary 2 tells us that  $\overline{x}$  exists and is non-constant provided that:

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or

$$T \in \left(\frac{2\pi}{\omega}, \frac{2\pi}{b_{\infty}}\right) . \tag{16}$$

*Proof.* The spectrum of  $\Lambda$  is  $\frac{2\pi}{T}Z + a_{\infty}$ . The largest negative eigenvalue  $\lambda$  is given by  $\frac{2\pi}{T}k_o + a_{\infty}$ , where

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Hence:

$$k_o = E\left[-\frac{T}{2\pi}a_\infty\right] \ . \tag{18}$$

The condition  $\gamma < -\lambda < \delta$  now becomes:

$$b_{\infty} - a_{\infty} < -\frac{2\pi}{T} k_o - a_{\infty} < \omega - a_{\infty} \tag{19}$$

which is precisely condition (14).

**Lemma 1.** Assume that H is  $C^2$  on  $\mathbb{R}^{2n} \setminus \{0\}$  and that H''(x) is non-degenerate for any  $x \neq 0$ . Then any local minimizer  $\widetilde{x}$  of  $\psi$  has minimal period T.

*Proof.* We know that  $\widetilde{x}$ , or  $\widetilde{x} + \xi$  for some constant  $\xi \in \mathbb{R}^{2n}$ , is a T-periodic solution of the Hamiltonian system:

$$\dot{x} = JH'(x) \ . \tag{20}$$

There is no loss of generality in taking  $\xi = 0$ . So  $\psi(x) \ge \psi(\widetilde{x})$  for all  $\widetilde{x}$  in some neighbourhood of x in  $W^{1,2}\left(\mathbb{R}/T\mathbb{Z};\mathbb{R}^{2n}\right)$ .

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

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

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

$$i_T(\widetilde{x}) = i_{kT/k}(\widetilde{x}) \ge ki_{T/k}(\widetilde{x}) + k - 1 \ge k - 1 \ge 1.$$
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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  $x_T$ ,  $T \in (2\pi\omega^{-1}, 2\pi b_{\infty}^{-1})$  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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1945 A.D.	2,300,000,000
1980 A.D.	4,400,000,000

**Theorem 1 (Ghoussoub-Preiss).** Assume H(t,x) is  $(0,\varepsilon)$ -subquadratic at infinity for all  $\varepsilon > 0$ , and T-periodic in t

$$H(t, \cdot)$$
 is convex  $\forall t$  (23)

$$H(\cdot, x)$$
 is  $T$ -periodic  $\forall x$  (24)

$$H(t,x) \ge n(\|x\|)$$
 with  $n(s)s^{-1} \to \infty$  as  $s \to \infty$  (25)

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

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

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:

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

where  $f_o := T^{-1} \int_0^T f(t) dt$ . For instance,

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

where  $\delta_k$  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  $(A_{\infty},B_{\infty})$ -subquadratic at infinity if there exists a function N(t,x) such that:

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

$$\forall t$$
,  $N(t,x)$  is convex with respect to  $x$  (33)

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

$$\exists c \in \mathbb{R} : H(t,x) \le \frac{1}{2} (B_{\infty}(t)x, x) + c \quad \forall x .$$
 (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  $(a_{\infty}, b_{\infty})$ -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

$$H(t,x) = \frac{1}{2}k \|k\|^2 + \|x\|^{\alpha}$$
(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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- Rabinowitz, P.: On subharmonic solutions of a Hamiltonian system. Comm. Pure Appl. Math. 33 (1980) 609–633

### Hamiltonian Mechanics2

Ivar Ekeland<sup>1</sup> and Roger Temam<sup>2</sup>

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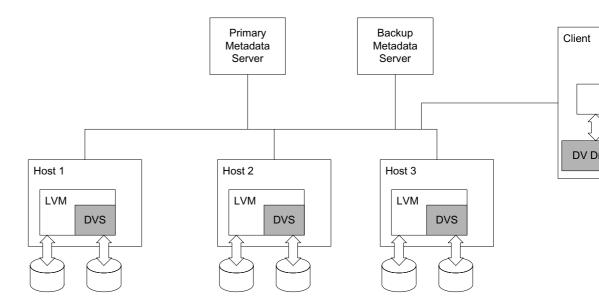


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50 A.D.	200,000,000
1650 A.D.	500,000,000
1945 A.D.	2,300,000,000
1980 A.D.	4,400,000,000

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:

$$p \ge p_o \Rightarrow x_{pk} \ne x_k$$
 (28)

Example 2 (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:

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

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

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

where  $\delta_k$  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 2.** 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  $(A_{\infty}, B_{\infty})$ -subquadratic

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

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

$$\forall t$$
,  $N(t,x)$  is convex with respect to  $x$  (33)

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

$$\exists c \in \mathbb{R} : H(t,x) \le \frac{1}{2} (B_{\infty}(t)x, x) + c \quad \forall x .$$
 (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  $(a_{\infty}, b_{\infty})$ -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

$$H(t,x) = \frac{1}{2}k \|k\|^2 + \|x\|^{\alpha}$$
(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 1985, 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 1981 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. 1982 and Tarantello, G. 1983) 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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## Subject Index

Absorption 327 Brillouin-Wigner perturbation theory Absorption of radiation 289-292, 299, 203 300 Cathode rays 8 Actinides 244 Causality 357–359 Aharonov-Bohm effect 142–146 Center-of-mass frame 232, 274, 338 Angular momentum 101–112 Central potential 113-135, 303-314 - algebraic treatment 391-396 Centrifugal potential 115–116, 323 Angular momentum addition 185–193 Characteristic function 33 Angular momentum commutation rela-Clebsch-Gordan coefficients 191-193 tions 101 Cold emission 88 Angular momentum quantization 9–10, 104 - 106Combination principle, Ritz's 124 Angular momentum states 107, 321, Commutation relations 27, 44, 353, 391 Commutator 21-22, 27, 44, 344 391 - 396Compatibility of measurements 99 Antiquark 83  $\alpha$ -rays 101–103 Complete orthonormal set 31, 40, 160, Atomic theory 8-10, 219-249, 327 Average value Complete orthonormal system, see (see also Expectation value) 15–16, 25, 34, Complete orthonormal set Complete set of observables, see Complete 37, 357 set of operators Baker-Hausdorff formula 23 Balmer formula 8 Eigenfunction 34, 46, 344–346 Balmer series 125 - radial 321 Baryon 220, 224 -- calculation 322 - 324Basis 98 EPR argument 377–378 Basis system 164, 376 Exchange term 228, 231, 237, 241, 268, Bell inequality 379–381, 382 272 Bessel functions 201, 313, 337 - spherical 304–306, 309, 313–314, 322 f-sum rule 302 Bound state 73-74, 78-79, 116-118, 202, Fermi energy 267, 273, 306, 348, 351  $H_2^+$  molecule 26 Boundary conditions 59,70Half-life 65 Bra 159 Breit-Wigner formula 80, 84, 332 Holzwarth energies 68