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Adiabatic Theory, Liapunov Exponents, and Rotation Number for Quadratic Hamiltonians

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We consider the adiabatic problem for general time-dependent quadratic Hamiltonians and develop a method quite different from WKB. In particular, we apply our results to the Schrödinger equation in a strip. We show that there exists a first regular step (avoiding resonance problems) providing one adiabatic invariant, bounds on the Liapunov exponents, and estimates on the rotation number at any order of the perturbation theory. The further step is shown to be equivalent to a quantum adiabatic problem, which, by the usual adiabatic techniques, provides the other possible adiabatic invariants. In the special case of the Schrödinger equation our method is simpler and more powerful than the WKB techniques.

KEY WORDS: Adiabatic invariants; Liapunov exponents; rotation number; localization; Schrödinger equation; integrated density of states; random potentials.

1. INTRODUCTION

In this paper we consider the quadratic Hamiltonian systems

$$h(p, q; t) = \tfrac{1}{2}(p, q \,|H|\, p, q) \tag{1}$$

where H is a real, quadratic form (that is, a $2n \times 2n$ symmetric matrix) depending on time. Thus, the equations of motion are provided by

$$dp/dt = -\partial h/\partial q, \qquad dq/dt = \partial h/\partial p$$

or, equivalently, if we set $u = (p, q)$,

$$du/dt = JHu \tag{2}$$

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where J is the skew-symmetric matrix

$$J=\begin{pmatrix} 0 & -Id \\ Id & 0 \end{pmatrix}$$

Furthermore, we will always assume that H is strictly positive, and we look at the case where H is a smooth, slowly varying family of quadratic forms $H(\varepsilon t)$ for which ε is a small parameter. A particular choice for this family yields the system of second-order differential equations

$$\ddot{u}+A(\varepsilon t)u=0 \tag{3}$$

where $A(\varepsilon t)$ is an $n\times n$ (strictly positive) symmetric matrix depending slowly on time. This case corresponds, for instance, to a set of slowly varying coupled harmonic oscillators. Many results have already been obtained in the framework of the theory of adiabatic invariants. One usually assumes that $A(t)$ is k-times differentiable and has definite limits at $\pm\infty$. Then, under the hypothesis that the eigenvalues of A are never degenerate,[1] one can show that the action variables of the Hamiltonian problem are good invariants in the sense that their total variation in time is at most of order ε^k. This kind of result is very special to the case of linear equations (or quadratic Hamiltonians) except in the one-dimensional case, where Neishtadt[2] has obtained analogous results for general nonlinear systems. In a previous paper[3] we showed that the results in the one-dimensional linear case allow us to get rigorous bounds for the exponential increase of solutions of (3) when we do not assume asymptotic limits for A. In particular, if $A(t)$ is an ergodic differentiable process, we can get upper bounds for the Liapunov exponent associated with (3). We refer to Ref. 3 for applications of these results to the Schrödinger equation: asymptotic width of the gaps, estimation of the integrated density of states. The present paper develops in this case a more general and simpler method than the WKB machinery. In this paper we extend our results to $n>1$. Let us stress that, in contrast with Ref. 1, we do not require that the eigenvalues of A are not degenerate, and we deal with general Hamiltonian systems as in (1). Of course, we do not assert that the n invariants obtained in Ref. 1 exist in general. We only prove that their sum is always an adiabatic invariant and this is sufficient to provide an upper bound for the rate of exponential increase of any solution of (1).

Equation (2) yields linear symplectic motion. The main idea of this paper is to carry out local (in time) symplectic changes of variables in order to simplify this equation. This idea is rather familiar in the study of dynamical systems, but unusual in the study of linear differential equations (for the Schrödinger equation one usually deals with the WKB method, which attempts to solve directly this equation). The linear symplectic group is the set of matrices S satisfying $S^TJS = J$; this set acts on the set of the quadratic forms $H \to S^THS$. Furthermore, any C^1 family $H(t)$ of quadratic, strictly positive Hamiltonians is mapped, through a C^1 family of canonical transforms $S(t)$, onto the family $H'(t) = S^THS + S^TJ\,dS/dt$. We can now state our basic theorem:

Theorem 1. Let $H(t)$ be a family of quadratic Hamiltonians satisfying the following properties:

(i) There exist strictly positive constants K_1, K_2 such that

$$0 < K_1 \cdot I_d < H(t) < K_2 \cdot I_d$$

(ii) The family is C^k and all its derivatives are uniformly bounded (later we will say "uniformly C^k").

Then, for sufficiently small ε, the adiabatic problem $H(\varepsilon t)$ is conjugated through a uniformly bounded family of symplectic transforms with the following Hamiltonian problem:

$$H'(\varepsilon t) = H^-(\varepsilon t) + \varepsilon^k h(\varepsilon t)$$

where h is uniformly bounded and

$$H^-(\varepsilon t) = H_0^- + \varepsilon H_1^- + \varepsilon^2 H_2^- + \cdots + \varepsilon^{k-1} H_{k-1}^-$$

where H_i^- belongs to the space E^- of J-commuting matrices and is uniformly C^{k-i}.

The dominant term in H' is the first one and it belongs to E^-. But, for any element H^- of E^-, JH^- is a generator of symplectic rotation in R^{2n}. Then, up to order ε^k, the norm of u is a trivial invariant of Eq. (2). This proves the existence of an adiabatic invariant in the C^k case. Theorem 1 is obtained by using repeatedly the following Proposition:

Proposition 1. There exists an analytic map from the set of strictly positive quadratic forms into the symplectic transform $H \to S_H$ such that $S_H^T H S_H$ belongs to the set E^- of quadratic forms commuting with J.

Comment. Below we give an explicit construction for this analytic map.

Theorem 1 yields that up to order ε^k the initial problem is equivalent to a problem of quantum adiabatic invariants on an n-dimensional Hilbert space. This class of problems is more familiar to physicists and simpler since it involves the unitary group instead of the symplectic group. In any case, at this step, the problem is reduced to a first-order n-dimensional linear system. The usual perturbative theorems[4,5] provide the results of Ref. 1 with some slight extensions.

In the special case where one assumes that $H(t)$ is asymptotically constant, Theorem 1 allows us to exhibit an explicit adiabatic invariant up to order ε^k: this is an extension to general (possibly degenerate) Hamiltonians of parts of the results of Ref. 1.

The following corollary provides a general asymptotic behavior for slowly varying Hamiltonians (without particular assumptions at infinity):

Corollary 1. Let $H(t)$ satisfy the hypotheses of Theorem 1. Then for sufficiently small ε any solution u of the adiabatic problem

$$du/dt = JH(\varepsilon t)u$$

satisfies

$$\limsup_{t \to \infty} \frac{1}{t} |\log \|u(t)\|| < C\varepsilon^k$$

In particular, if $H(t)$ is an ergodic differentiable process, this corollary provides an upper bound for the Liapunov exponents of (1).

We apply our results to the analysis of the eigenvalue problem associated with the generalized Schrödinger operator:

$$H\Psi = -d^2\Psi/dx^2 + A(x)\Psi \tag{4}$$

where Ψ is an n-component vector and A an $n \times n$ symmetric matrix. Then, the behavior of the eigenfunctions associated with large eigenvalues is equivalent to a degenerate problem of type (1). Our results yield an upper bound on the rate of decrease of eigenfunctions associated with (4) in the limit of large eigenvalues.

Finally, we introduce a rotation number for any continuous family of symplectic transforms and we prove, in the limit of adiabatic linear Hamiltonian problems, the following corollary:

Corollary 2. Let $H(t)$ satisfy the hypotheses of Theorem 1. Then for sufficiently small ε the rotation number α of the adiabatic problem

$$du/dt = JH(\varepsilon t)u$$

is given by

$$\alpha = \limsup_{t \to \infty} \frac{1}{2\pi t} \int_0^t \operatorname{Tr} H^-(\varepsilon t)\, dt + O(\varepsilon^k)$$

where H^- is provided by Theorem 1.

In the case of the Schrödinger operator (4), this corollary provides an estimate of the integrated density of states for large energies.

2. PROOF OF PROPOSITION 1

We will use the following splitting of the set E of the quadratic forms into E^+ and E^-:

$$E^+ = \{H; JH + HJ = 0\} \tag{5}$$

$$E^- = \{H; JH - HJ = 0\} \tag{6}$$

These two spaces satisfy $E = E^+ \oplus E^-$ and thus any quadratic form H can be written

$$H = H^+ + H^- \tag{7}$$

where $H^+ = \frac{1}{2}(H + JHJ)$ and $H^- = \frac{1}{2}(H - JHJ)$ are the projections of H associated with the splitting. The general form of an element in E^+ is

$$H^+ = \begin{pmatrix} A & B \\ B & -A \end{pmatrix} \tag{8}$$

where A and B are symmetric. Any element in E^- has the form

$$H^- = \begin{pmatrix} A & B \\ -B & A \end{pmatrix} \tag{9}$$

where A is symmetric and B is skew-symmetric. In general the orthogonal projection onto E^- is not a symplectic transform. We have to find a linear symplectic matrix S_H such that $S_H^T H S_H$ belongs to E^-, that is

$$S_H^T H S_H = -J S_H^T H S_H J$$

Since S_H is symplectic, this is equivalent to

$$S_H S_H^T H S_H S_H^T = -JHJ$$

The matrix $S_H S_H^T$ is positive symmetric and symplectic (S_H^T is symplectic as soon as S_H is symplectic). Now we assume that H is strictly positive, so that if we use the change of variables $S_H S_H^T = H^{-1/2} K H^{-1/2}$ then K has to be positive symmetric and to satisfy

$$K^2 = -H^{1/2} JHJ H^{1/2} \tag{10}$$

The unique solution is $K = (-H^{1/2} JHJ H^{1/2})^{1/2}$. Indeed, the left-hand side of (10) is a positive symmetric matrix. This yields

$$S_H S_H^T = H^{-1/2} (-H^{1/2} JHJ H^{1/2})^{1/2}\, H^{-1/2} \tag{11}$$

We first have to check that $S_H S_H^T$ is actually a symplectic matrix. Setting $N = H^{1/2} J H^{1/2}$, we have to check that

$$H^{-1/2}(N^T N)^{1/2} N^{-1} (N^T N)^{1/2} H^{-1/2} = -J \tag{12}$$

that is

$$|N|\, N^{-1}\, |N| = N \tag{13}$$

where $|N|$ stands for $(N^T N)^{1/2}$. But since N is a normal operator, it commutes with $|N|$ and (13) is equivalent to $|N|^2 = -N^2$, which is satisfied since N is skew-symmetric. Thus, (11) defines a symplectic solution $S_H S_H^T$ depending analytically on H (as soon as $H > 0$), and the last step is to find a symplectic solution S_H depending analytically on $S_H S_H^T$. One can easily check that $(S_H S_H^T)^{1/2}$ is still symplectic and thus provides a convenient solution. But, in the proof of Corollary 2, we shall need a "triangular" solution of the form

$$S_H = \begin{pmatrix} a & 0 \\ b & a^{T-1} \end{pmatrix}$$

where a and b are $n \times n$ matrices satisfying $a^T b = b^T a$, to ensure that S_H is symplectic. Thus, we have to solve the following equation in a and b:

$$S_H S_H^T = \begin{pmatrix} A & B \\ B^T & D \end{pmatrix} = \begin{pmatrix} aa^T & ab^T \\ ba^T & (aa^T)^{-1} + bb^T \end{pmatrix}$$

where A and D are strictly positive symmetric $n \times n$ matrices (since $S_H S_H^T$ is symmetric positive) and B is any $n \times n$ matrix satisfying

$$AB^T = BA \tag{14}$$

$$B^T D = DB \tag{15}$$

$$AD - B^2 = Id \tag{16}$$

Let us first notice that D is uniquely determined by A and B, and it is thus sufficient to solve

$$A = aa^T$$

$$B^T = ba^T$$

A regular solution is provided by

$$a = A^{1/2} \tag{17}$$

$$b = B^T A^{-1/2} \tag{18}$$

since Eq. (14) ensures that S_H is symplectic. Furthermore, it is important for the study of the rotation number that our "triangular" symplectic matrices form a group, which is not the case for symmetric ones. Thus, iterating our symplectic transforms still provides "triangular" symplectic transforms.

3. PROOF OF THEOREM 1

Let us consider a k-times differentiable Hamiltonian $H(t)$ satisfying the hypotheses of Theorem 1. Using the variable $\tau = \varepsilon t$ and the transform of Proposition 1, we get

$$H'(\varepsilon t) = S_H^T H S_H + \varepsilon S_H^T J\, dS_H/d\tau \tag{19}$$

$$= H_0^- + \varepsilon h_1 \tag{20}$$

The first term is C^k and lies in E^-, and the second one is C^{k-1} and of order ε: this is exactly the announced result for $k=1$. We now proceed recursively, and we assume that after p transformations $(p<k)$ the Hamiltonian is given by

$$H(\varepsilon t) = H_0^- + \varepsilon H_1^- + \varepsilon^2 H_2^- + \cdots + \varepsilon^{p-1} H_{p-1}^- + \varepsilon^p h_p \tag{21}$$

where H_i^- lies in E^- and is uniformly C^{k-i}, and h_p is uniformly C^{k-p}. Let us now recall that the symplectic transform S_H depends analytically on H and is the identity for any H in E^-. Thus, for H given by (22), S_H may be written as

$$S_H = Id + \varepsilon^p S_H(\varepsilon t) \qquad \text{where } S_H \text{ is uniformly } C^{k-p} \tag{22}$$

Then, $S_H^T H S_{H^-} H$ is of order ε^p and uniformly C^{k-p}, and $S_H^T H S_H$ belongs to E^-. Thus, we have

$$S_H^T H S_H = H_0^- + \varepsilon H_1^- + \varepsilon^2 H_2^- + \cdots + \varepsilon^p H_p^- \tag{23}$$

$$H'(\varepsilon t) = S_H^T H S_H + \varepsilon^{p+1} S_H^T J\, ds_H/d\tau$$

$$= H_0^- + \varepsilon H_1^- + \varepsilon^2 H_2^- + \cdots + \varepsilon^p H_p^- + \varepsilon^{p+1} h_{p+1} \tag{24}$$

where H_p^- is in E^- uniformly C^{k-p}, and h_{p+1} is uniformly C^{k-p-1}. While $p<k$, we can iterate this procedure in order to get the result announced in Theorem 1.

Theorem 1 allows us, through a uniformly bounded family of symplectic transforms, to translate the initial problem (2) into a form that provides

$$d\,\|u\|^2/dt = 2\varepsilon^k (u, Jh(\varepsilon t) u) \tag{25}$$

Thus

$$d\,\|u\|^2/dt \leqslant \varepsilon^k C\,\|u\|^2 \tag{26}$$

This provides the bounds of Corollary 1 in the new coordinates; these asymptotic bounds remain true through the bounded symplectic change of variables that goes back to the initial coordinates. This ends the proof of Corollary 1.

4. COMMENT: REDUCTION TO THE QUANTUM ADIABATIC THEORY

Let H satisfy the hypotheses of Theorem 1. We have proven that up to order ε^k this problem is equivalent to a new Hamiltonian H' lying in E^-:

$$H' = H_0^- + \varepsilon H_1^- + \varepsilon^2 H_2^- + \cdots + \varepsilon^{k-1} H_{k-1}^-$$

where H_i^- is uniformly C^{k-i}. Thus, H' commutes with J and in particular with the orthogonal projector $P = (1 - iJ)/\sqrt{2}$ and we have

$$P\,du/dt = PJH'u$$

that is,

$$dPu/dt = JPH'Pu = iPH'Pu \tag{27}$$

where we have used $JP = iP$. More precisely, if H' is given by Eq. (9), setting $\Psi = p + iq$ and $\mathscr{H} = A + iB$, then Eq. (27) is equivalent to the quantum time-dependent Hamiltonian problem:

$$i\,d\Psi/dt = \mathscr{H}(\varepsilon t)\Psi$$

where $\mathscr{H}$ is a self-adjoint operator.

In the special case where the distance between eigenvalues of $\mathscr{H}$ is uniformly bounded from below, we can apply the usual techniques (by successive diagonalizations), which yields the results of Ref. 1.

5. APPLICATION TO THE SCHRÖDINGER EQUATION

Let us now consider a degenerate problem which occurs in the study of the generalized Schrödinger operator (4) and look at the eigenvalue problem in the limit of large eigenvalues:

$$-d^2\Psi/dx^2 + A(x)\Psi = E\Psi \tag{28}$$

Setting $\varepsilon = 1/\sqrt{E}$, $x = \varepsilon t$, and $u(t) = \Psi(x)$, we get

$$d^2u/dt^2 + [1 - \varepsilon^2 A(\varepsilon t)]u = 0 \tag{29}$$

The corresponding quadratic form for the classical Hamiltonian problem in the variables $(p, q) = (du/dt, u)$ is defined by

$$H = \begin{pmatrix} 1 & 0 \\ 0 & 1 - \varepsilon^2 A \end{pmatrix} \tag{30}$$

This problem is completely degenerate, since all the eigenvalues of H go to 1 as ε goes to zero. The usual techniques do not apply and actually there is only one adiabatic invariant. We can apply our results. In this case the first step is especially simple and gives rises to a symplectic transform S:

$$S = \begin{pmatrix} [1 - \varepsilon^2 A]^{1/4} & 0 \\ 0 & [1 - \varepsilon^2 A]^{-1/4} \end{pmatrix} \tag{31}$$

Finally, assuming that A is uniformly C^k, we get

$$\limsup 1/|t| \log \|u\| \leqslant C\varepsilon^{k+2} \tag{32}$$

Then

$$\limsup 1/|x| \log(\|\Psi'(x)\|^2 + \|\Psi(x)\|^2 \leqslant CE^{(k+1)/2} \tag{33}$$

We refer to Ref. 3 for applications to localization and asymptotic behavior of the gaps for Eq. (28).

6. THE ROTATION NUMBER

Generalization of Sturm–Liouville theory has already been considered by various authors. The rotation number for general second-order differential equations has been roughly defined in Ref. 6. Ruelle[7] defined the rotation number for a family of symplectic transform and in a companion paper[8] we give a different proof of it. Thus, we just recall some facts about it. In the following we denote by $U(n)$ the unitary group, that is, the intersection of the symplectic and the orthogonal group (or equivalently the group of the symplectic matrices commuting with J). A unitary operator U can be written as

$$U = \begin{pmatrix} a & b \\ -b & a \end{pmatrix} \tag{34}$$

where $a+ib$ is unitary in the usual sense. Let L be the set of Lagrangian subspaces (n-dimensional spaces isotropic with respect to the bilinear form J). If P and P' belong to L, then there exists a unitary operator U mapping P onto P'. This operator is defined up to an element of $O(n)$, that is, an element of $U(n)$ with $b=0$. Thus, to any pair (P, P') we can associate a unique element of the unit circle S^1 defined by $\det(a+ib)^2$. This definition is convenient since it is invariant by the subgroup $O(n)$ and this element of S^1 can be seen as an "angle" between the two Lagrangian spaces P and P'. Notice that a symplectic matrix maps a Lagrangian space onto a Lagrangian space. Now, given a continuous family $S(t)$ of symplectic matrices and a Lagrangian space P, we define the winding number of $S(t)$ with respect to P for t in $[0, t_0]$ as the total variation of the angle between P and $S(t)P$ until $t=t_0$. The rotation number is then defined as the limit (if it exists, or, say, the upper limit in general cases) of the winding number divided by $2\pi t_0$. The important point is that the winding number is "almost independent" of the Lagrangian space P, so that the rotation number becomes independent of the Lagrangian plane P. Furthermore, if $S(t)$ is given by

$$S=\begin{pmatrix} A & B \\ C & D \end{pmatrix} \tag{35}$$

then we prove that the winding number of the Lagrangian plane P_0 defined by $p=0$ is just provided by the winding number of the unitary matrix $(D-iB)^{-1}(D+iB)$. Thus, a convenient explicit formula for the rotation number α is

$$\alpha=\limsup_{T\to\infty} \operatorname{Im}(2\pi T)^{-1} \int \log(\det[(D-iB)^{-1}(D+iB)] \tag{36}$$

Remark. It is known that the fundamental group of linear symplectic group is $\mathbb{Z}$ and that this group is in fact provided by the fundamental group of $U(n)$, which is induced by the square determinant. Thus, we are looking at the rotation number in the symplectic group due to the fact that the π_1 of this group is $\mathbb{Z}$. This is in fact the property that Ruelle used to defined the rotation number. Finally, this shows that we have defined the unique possible winding number.

Now, $H(t)$ being given, we can consider the symplectic solution $S(t)$ of the adiabatic problem:

$$dS(t)/dt=JH(\varepsilon t)\,S(t), \qquad S(0)=1 \tag{37}$$

and look at the rotation number $\alpha(\varepsilon)$. The first point is to prove that using the symplectic change of variables of Theorem 1 does not affect the rotation number. This is obvious since our symplectic transforms are "triangular" and thus leave the plane P_0 invariant. The second step is to estimate the rotation number when the Hamiltonian is $H = H^- + \varepsilon H^+$. Then (41) provides

$$d(D + iB)/dt = (N - iM)(D + iB) + \varepsilon(Q + iP)(D - iB) \tag{38}$$

where

$$H^- = \begin{pmatrix} M & N \\ -N & M \end{pmatrix} \tag{39}$$

$$H^+ = \begin{pmatrix} P & Q \\ Q & -Q \end{pmatrix} \tag{40}$$

That is,

$$\begin{aligned} &\frac{d}{dt} \log \det[(D - iB)^{-1} (D + iB)] \\ &\qquad = 2i \operatorname{Tr} M + 2\varepsilon \operatorname{Im}[\operatorname{Tr}(Q + iP)(D - iB)(D + iB)] \\ &\qquad = i \operatorname{Tr} H^- + O(\varepsilon) \end{aligned} \tag{41}$$

Equation (41) follows from the fact that $(D - iB)/(D + iB)$ is unitary.

We end this section with an application to the Schrödinger operator. Let us consider the self-adjoint Schrödinger operator with Neumann boundary conditions at 0 and X, that is, $\Psi'(0) = \Psi'(x) = 0$. The eigenvalues of this operator correspond to the values of E in (28) such that the image of the Lagrangian space $\Psi' = 0$ at $x = 0$ possesses a nonzero intersection with itself at $x = X$. This means that the unitary operator $U = (D - iB)^{-1} (D + iB)$ has an eigenvalue equal to 1. Furthermore, it is known[6] that the argument of the eigenvalues of U increases continuously with E. Thus, the winding number (divided by 2π) of the Lagrangian space $\Psi' = 0$ provides the number of eigenvalues of the Schrödinger operator in $[0, X]$. The limit of this number divided by $2\pi X$ (whenever it exists) is the so-called integrated density of states. As we have claimed, it does not depend on the boundary conditions and is the rotation number of the eigenvalue equation. Finally, we mention that the convergence of these numbers is physically a weak assumption and occurs as soon as we assume some stationarity property for the problem. The natural framework is then the ergodic theory and has already been extensively studied.

REFERENCES

1. M. V. Fedoryuk, *Equations Differentielles* **12**:6 (1976).
2. A. I. Neishtadt, *Prikl Matem. Mekhan.* **45**:80 (1981).
3. F. Delyon and P. Foulon, *J. Stat. Phys.* **45**:41 (1986).
4. T. Kato, *Phys. Soc. Jpn.* **5** (1950).
5. M. Berry, *Proc. R. Soc. A* **392**:45 (1984).
6. F. V. Atkinson, *Discrete and Continuous Boundary Problems* (Academic Press, 1964).
7. D. Ruelle, *Ann. Inst. H. Poincaré Phys. Théor.* **42**:109 (1985).
8. F. Delyon and P. Foulon, Complex entropy for dynamical systems, Preprint, Ecole Polytechnique.

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