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Adiabatic Invariants and Asymptotic Behavior of Lyapunov Exponents of the Schrödinger Equation

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We give an upper bound for the high-energy behavior of the Lyapunov exponent of the one-dimensional Schrödinger equation. We relate this behavior to the diffrentiability properties of the potential. As an application, this result provides an upper bound for the asymptotic length of the gaps of the Schrödinger equation.

KEY WORDS: Adiabatic invariants; Schrödinger equation; Lyapunov exponents; localization; random potentials.

1. INTRODUCTION

We study the high-energy behavior of the one-dimensional Schrödinger equation. Although we do not suppose that the potential admits definite limits at infinity, we prove an adiabatic theorem which provides bounds on the growth rate of the solutions of the Schrödinger equation. In particular, when the Lyapunov exponent exists, we bound it in terms of the energy. This situation is of particular interest in solid-state physics, where the potential is supposed to obey some homogeneity condition; it may be periodic, in which case we bound the Lyapunov exponent in the gaps and consequently the length of the gaps (Remark 4). The potential may also be given as a random process, for instance, in the theory of disordered systems; in this later case the Schrödinger operator may (and often does) present a spectral resolution in term of exponentially localized eigenvectors: our results provide a bound on this exponential decay rate.

We shall prove the following theorem, which is, in the linear case, an extension of a Neishtadt's adiabatic theorem[(1)]:

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Theorem. Let $\Psi(x)$ be a real function satisfying the Schrödinger equation on $\mathbb{R}$:

$$-d^2\Psi/dx^2 + V(x) \cdot \Psi(x) = E\Psi(x) \tag{1}$$

where V and all its k first derivatives are continuous and uniformly bounded; then there exists a constant C such that for sufficiently large energy E

$$\limsup_{x \to \pm\infty} (2|x|)^{-1} |\log[\Psi^2(x) + \Psi'^2(x)]| < CE^{-(k+1)/2} \tag{2}$$

Furthermore, if V is analytic and uniformly bounded in a strip around the real axis, then $CE^{-(k+1)/2}$ may be replaced by $C\exp(-C'E^{1/2})$.

Remark 1. In various cases one knows the limit of the left-hand side of (2) to exist (for instance, with probability one if V is a random ergodic process) and to be the so-called Lyapunov exponent. Thus (2) in these cases is a rigorous upper bound for the Lyapunov exponent in the high-energy limit. This in turn provides the lower bound $E^{(k+1)/2}$ for the localization length of the eigenstates of (1).

Remark 2. This special case of a linear second-order differential equation has been studied, but in a different situation in relation to the WKB approach when the potential admits defined limits at infinity. At the opposite our situation can recover the case of an infinite number of turning points in the WKB method.

Remark 3. We expect that the bound proven in this paper provides in many cases the exact asymptotic behavior for the Lyapunov exponent. Furthermore, this behavior is already known when V is only uniformly bounded: the Lyapunov exponent is bounded by $CE^{-1/2}$.

Remark 4. Let us consider a Schrödinger equation (1) with a periodic potential V. It is well known that the spectrum consists of a sequence of energy bands in which any solution Ψ is bounded. Between these bands we (generically[(2)]) have gaps in which any Ψ increases exponentially at $+\infty$ or $-\infty$ at a rate we denote $\gamma(E)$. Furthermore, if $d(E)$ is the distance from E to the spectrum of the Schrödinger operator, by Simon's result (Ref. 3, Theorem 4.1) γ satisfies

$$d(E) \leqslant \gamma(E)^2 + D\gamma(E)(E^{1/2} + 1)$$

where D is a constant depending only on V. Thus, by our theorem the length L of a gap is bounded by $D'E^{-k/2}$ if V is C^k (in the sense given in the theorem) and by $e^{-\alpha\sqrt{E}}$ if V is analytic. In fact this bound does not require the periodicity of the potential and our result is the first one in this general frame. In others words, since the energy of the nth gap is of order n^2, the length L_n of the nth gap satisfies

$$L_n \leqslant D'' n^{-k} \text{ (resp. } e^{-\alpha n})$$

when V is C^k (resp. analytic). In the C^k periodic case an analogous result was already obtained[6] for even k and under Lipschitz conditions. The analytic periodic case was solved by Grigis.[7] In the very special case of the Mathieu equation, Avron and Simon[4] have obtained the exact behavior $L_n \sim n^{-n}$.

Equation (1) is equivalent to the equation of motion of a parametric oscillator. Thus, our results may be restated in terms of the theory of adiabatic perturbations of integrable Hamiltonian systems. Let us consider a family of Hamiltonians $H(p, q; \lambda)$, where p and q stand for the momentum and position variables and λ is a real parameter. For fixed λ the system is integrable and we denote by $I(\lambda)$ the action variable. Now let us suppose that λ is a slowly varying function of the time: $\lambda = \lambda(\varepsilon t)$; then one expects that the action variable I remains almost constant. For instance,[8] if one varies smoothly in time the frequency of harmonic oscillator, one expects the almost constancy of the action variable, that is, of the ratio $H(\lambda)/\omega(\lambda)$, where $\omega(\lambda)$ is the frequency of the oscillator. In that direction many exact results have been obtained (mainly) by Russian mathematicians. One can find useful references in Arnold's book[5]; we are especially indebted to the results obtained by Neishtadt.[1] In our case, taking into account the linearity of the problem, we can extend Neishtadt's results and bound the growth rate of the logarithm of the adiabatic invariant.

2. PROOF OF THE THEOREM

First we choose the new variable $t = E^{1/2}x$; then Eq. (1) becomes

$$-\Psi'' + V(tE^{-1/2})\, E^{-1}\Psi = \Psi \tag{3}$$

Now (3) is equivalent to the Hamiltonian system

$$H_0(p, q, t) = p^2 + [1 - V(\varepsilon t)\, \varepsilon^2]\, q^2 \tag{4}$$

where $\varepsilon = E^{-1/2}$, $q = \Psi$, and $p = \Psi'$. For "fixed t" the system is integrable in terms of the action–angle variables $I = H_0/\omega$ and $\tan \varphi = \omega q/p$, where ω is the frequency $(1 - V\varepsilon^2)^{1/2}$. Notice that I is just $[(d\Psi/dx)^2/E + \omega^2\Psi^2]/\omega$, which is equivalent to the argument of the logarithm in (2) in the sense

$$\lim_{x \to \pm\infty} \sup\ 1/|x| \log(\Psi^2 + \Psi'^2) = \lim_{x \to \pm\infty} \sup\ 1/|x| \log I \tag{5}$$

The new Hamiltonian is

$$H(I, \varphi; t) = I[\omega + (\omega'/2\omega) \sin 2\varphi] = I\omega[1 + f(\varphi, t)] \tag{6}$$

where ω' is of order ε^3. We suppose there that V is differentiable and satisfies $E \gg |V|_\infty$. At this step, we have

$$dI/dt = -\partial H/\partial\varphi = -|\omega'/\omega \cos 2\varphi| \tag{7}$$

that is,

$$d \log I/dt = -\omega'/\omega \cos 2\varphi \tag{8}$$

which provides the announced result as soon as V is C^1. Now for a C^k $(k \geqslant 2)$ potential the proof relies on the following lemma:

Lemma 1. Consider the Hamiltonian system

$$H(I, \varphi; t) = I\omega(\varepsilon t)[1 + \varepsilon^p f(\varphi, \varepsilon t)] \tag{9}$$

where ω and f as their nth first derivatives (with respect to φ and εt) are uniformly bounded and C^1 with respect to φ for $\varphi \in [0, 2\pi]$ and $t \in \mathbb{R}$, and f has zero mean value with respect to φ for all t. Then for ε in a neighborhood of 0 there exists a canonical transform that maps (9) onto the following system:

$$H_1(I_1, \varphi_1; t) = I_1 \omega_1(\varepsilon t)[1 + \varepsilon^{p+1} f_1(\varphi_1, \varepsilon t)] \tag{10}$$

where ω_1 and f_1 as their $(n-1)$th first derivatives are uniformly bounded and C^1 with respect to φ_1 and f_1 has zero mean value with respect to φ for all t.

Proof of Lemma 1. Following Neishtadt's idea, we introduce the generating function of the canonical transform $S(I_1, \varphi)$:

$$S(I_1, \varphi) = I_1\left[\varphi - \int_{H=\text{const}}^{\varphi} \varepsilon^p f(\varphi, \varepsilon t)\, d\varphi\right] \tag{11}$$

which provides

$$I = \partial S(I_1, \varphi)/\partial\varphi = I_1[1 - \varepsilon^p f(\varphi, \varepsilon t)] \tag{12}$$

$$\varphi_1 = \partial S(I_1, \varphi)/\partial I_1 = \varphi - \int_{H=\text{const}}^{\varphi} \varepsilon^p f(\varphi, \varepsilon t)\, d\varphi \tag{13}$$

We have to notice that φ_1 is a function of φ and t only, since S is linear with respect to I_1. For small ε these changes of variables are convenient by the implicit functions theorem: (13) shows that $d\varphi_1/d\varphi$ (for fixed t) uniformly goes to one as ε goes to zero. Furthermore, $d\varphi_1/d\varphi$ is a C^n function (with respect to φ). The new Hamiltonian $H_1(I_1, \varphi_1, t)$ is

$$H_1(I_1, \varphi_1, t) = H(I_1, \varphi_1, t) - \partial S/\partial t = I_1 \omega(1 + \varepsilon^p f') \tag{14}$$

with

$$f' = -\varepsilon^p f^2(\varphi, \varepsilon t) + \omega^{-1} \int_{H=\text{const}}^{\varphi} [\partial f(\varphi', \varepsilon t)/\partial t] \, d\varphi' \tag{15}$$

$H_1(I_1, \varphi_1, t)$ is again defined as in (9) with a new function f' of order $\partial f/\partial t$, that is, εf. The $(n-1)$th first derivatives of f' with respect to t and φ_1 may be expressed in terms of the nth first derivatives of f with respect to t and φ. Thus, they are uniformly bounded and C^1 in φ; since for fixed t, φ_1 is a C^n function of φ, they are also uniformly C^1 in φ_1. In fact, to be convenient, f' should have zero mean value; this can be done by defining a new frequency ω_1:

$$\omega_1 = (\omega/2\pi) \oint d\varphi_1 \, (1 + \varepsilon^p f') \tag{16}$$

$H_1(I_1, \varphi_1, t)$ is now defined as in Lemma 1 with a function f_1 satisfying the required conditions. ∎

We now continue the main proof. Under the hypotheses of the theorem, the function f defined in (8) satisfies the hypotheses of Lemma 1 with $p = 3$ and $n = k - 1$. Thus, we may apply Lemma 1 a total of $k - 1$ times to obtain a Hamiltonian H_k:

$$H_k(I_k, \varphi_k; t) = I_k \omega_k(\varepsilon t)[1 + \varepsilon^{k+2} f_k(\varphi_k, \varepsilon t)] \tag{17}$$

The equation of motion for I is now

$$dI_k/dt = -I_k \omega_k \varepsilon^{k+2} \, \partial f_k/\partial \varphi_k \tag{18}$$

and yields

$$|\log I_k(t)| < C(k) \, \varepsilon^{k+2} \, |t| \tag{19}$$

Clearly, by (12), $|\log(I_k/I)|$ is uniformly bounded; thus

$$\begin{aligned} \lim \sup_{x \to \pm\infty} 1/|x| \, |\log I| &= \lim \sup_{t \to \pm\infty} 1/|\varepsilon t| \, |\log I_k| \\ &\leqslant C(k) \, \varepsilon^{k+1} \end{aligned} \tag{20}$$

Together with (5), this yields the announced result when V is C^k.

We now turn to the analytic case. We suppose V is bounded and analytic in a strip around the real axis; we are going to use the same canonical transforms as in the C^k case. Thus, now ω and f [defined as in (9) with $p=3$]) are bounded and analytic in a strip (R, r) around the real axis $\{\text{Im}(\varepsilon t)<R, \text{Im}(\varphi)<r\}$:

$$|\omega - 1| < \eta \qquad \text{if} \quad |\text{Im}(\varepsilon t)| < R \tag{21}$$

$$|f(\varphi, \varepsilon t)| < M \qquad \text{if} \quad |\text{Im}(\varepsilon t)| < R \quad \text{and} \quad |\text{Im}(\varphi)| < r \tag{22}$$

To pursue the iteration of the canonical transforms, we need the following lemma:

Lemma 2. Let us assume that ω and f in Lemma 1 satisfy (21) and (22); then ω_1 and f_1 are analytic in a strip $(R_1 < R, r_1 = r - \varepsilon^p M 2\pi)$ and satisfy.

$$|\omega_1 - 1| < \eta_1; \qquad |f_1(\varphi_1, \varepsilon t)| < M_1 \tag{23}$$

where η_1 and M_1 are given by

$$M_1 = \varepsilon^{p-1} M^2 + 2\pi M (1-\eta)^{-1} (R - R_1)^{-1} \tag{24}$$

$$\eta_1 = \eta + (1+\eta)\, \varepsilon^{p+1} M_1 \tag{25}$$

Proof of Lemma 2. The function f' is still defined by (15) and, for $(\varepsilon t, \varphi)$ in the strip $(R_1 < R, r)$, is bounded by

$$f' < \varepsilon^p M^2 + 2\pi M \varepsilon (1-\eta)^{-1} (R - R_1)^{-1} \tag{26}$$

The change of variable (13) is now analytic and the image of the strip $\{|\text{Im}(\varphi)| < r\}$ contains the strip $\{|\text{Im}(\varphi_1)| < r_1 = r - \varepsilon^p M 2\pi\}$. Thus, f' as a function of φ_1 is bounded in this strip by (26); hence, f_1 is bounded by $\varepsilon^{p-1} M^2 + 2\pi M (1-\eta)^{-1} (R - R_1)^{-1}$; the result for ω_1 follows easily. ∎

Now the end of the proof is straightforward: we iterate this procedure $N-1$ times, choosing $R_i - R_{i+1} = R/N$. At the first step η was of order $\varepsilon^2 M$. Let us suppose that (i) η will remain smaller than, say, 1/2 and (ii) the first term in the right-hand side of (24) will remain smaller than the second one. We will have to check (i) and (ii) later. Then inequalities (24) and (25) can be simplified:

$$\eta_{i+1} < \eta_i + 2\varepsilon^{4+i} M_{i+1} \tag{27}$$

$$M_{i+1} < 8\pi M_i N/R \tag{28}$$

Hence M_i (resp. η_i) is smaller than $(8\pi N/R)^i M$[resp. $\varepsilon^2 M + 16\pi M \varepsilon^4 N/(R - 8\pi N\varepsilon)$] as soon as $8\pi\varepsilon N/R < 1$. For $M\varepsilon^2$ sufficiently small and

$8\pi\varepsilon N/R < 1$ the previous hypotheses are thus satisfied and M_{N-1} is now bounded by $(8\pi N/R)^{N-1} M$. Now using (18), we have $dI_{N-1}/dt \sim I_{N-1}\varepsilon^{N+1}M_{N-1}N/R$; we see that the best estimate is provided by $N \sim 1/\varepsilon$ such that $\varepsilon^{N+1}M_{N-1}N/R \sim e^{-\alpha/\varepsilon}$. Once more, as in (9) and (10), we get that $\log I$ cannot increase (or decrease) faster than $te^{-\alpha/\varepsilon}$, which is the announced result going back to the variables Ψ, Ψ'. ∎

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REFERENCES

1. A. I. Neishtadt, *Prikl. Matem. Mekhan.* **45**:80 (1981).
2. H. P. McKean and E. Trubowitz, *Commun. Pure Appl. Math.* **29**:143 (1976).
3. B. Simon, *J. Funct. Anal.* **42**:347 (1981).
4. J. Avron and B. Simon, *Ann. Phys. (N.Y.)* **134**:76 (1981).
5. V. Arnold, *Chapitres supplémentaires de la théorie des équations différentielles ordinaires* (Mir, 1980).
6. V. Latzutkin and T. Parkratova, *Sov. Math. Dokl.* **15** (1974).
7. A. Grigis, Sur l'équation de Hill analytique, Séminaire Bony-Sjöstrand-Meyer 1984–1985, Centre de Mathématiques École Polytechnique, Palaiseau, France.
8. L. D. Landau and E. M. Lifschitz, *Classical Mechanics.*