Divergence of the Chaotic Layer Width and Strong Acceleration of the Spatial Chaotic Transport in Periodic Systems Driven by an Adiabatic ac Force

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We show for the first time that a weak perturbation in a Hamiltonian system may lead to an arbitrarily wide chaotic layer and fast chaotic transport. This generic effect occurs in any spatially periodic Hamiltonian system subject to a sufficiently slow ac force. We explain it and develop an explicit theory for the layer width, verified in simulations. Chaotic spatial transport as well as applications to the diffusion of particles on surfaces, threshold devices and others are discussed.

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The basic chaotic formation in perturbed Hamiltonian systems is a chaotic layer associated with a separatrix of the unperturbed (integrable) Hamiltonian system. Even in the simplest case, when the unperturbed Hamiltonian system is one-dimensional while the perturbation is time-periodic, both the transport within the layer and its structure on the Poincaré section, relating to the homoclinic tangle, are very complicated. At the same time, the boundaries of the layer are well defined as the last invariant curves which limit the layer from above and below in the energy scale, and may be accurately found in numerical simulations. For both theory and applications, one of the most important characteristics of the layer is its width in energy or in related quantities. It might be assumed that, if the perturbation is very weak, then the layer should necessarily be narrow. This natural assumption seems to be supported by numerous examples (e.g. 1, 2, 4, 5, 6, 10, 11). However, we show in the present Letter that the situation may drastically differ (Fig. 1) in a rather general case, namely for any spatially periodic system driven by a slow ac force: the upper energy boundary of the layer diverges as the frequency of the force goes to zero. We explain this, develop a theory and verify it by simulations. We also demonstrate that the chaotic transport in space may be very fast in the adiabatic case, on sufficiently long time-scales, and discuss some applications.

Before moving on to the detailed consideration, we comment on the relation to 10. It is shown in 10 that, for a system with adiabatically slowly pulsating parameters, the homoclinic tangle covers most of the range swept by the instantaneous separatrix. If the pulsation of parameters in 10 were weak, the range swept would be narrow. Our system essentially differs from that considered in 10 (our perturbation is not parametric) so the result of 10 cannot be directly applied to it. If nevertheless the result of 10 were formally generalized to our system, it would give that the homoclinic tangle in the adiabatic limit covered the whole phase space, thus hinting at a divergence of the chaotic layer width.

Periodic systems and ac forces are widespread in nature. An archetypal example is a pendulum driven by a weak single-harmonic ac force:

\[ \dot{q} = p, \quad \dot{p} = -dU_0/dq - \omega_0^2 \sin(\omega_ft) \equiv -dU/dq, \]
\[ U_0 \equiv U_0(q) = -\omega_0^2 \cos(q), \]
\[ U \equiv U(q,t) = U_0(q) + q\omega_0^2 \sin(\omega_ft), \quad h \ll 1. \]  

To get some insight into the physical origin of the phenomenon, and to obtain a qualitative explanation of Fig. 1, we first consider the strong adiabatic limit

\[ \epsilon \equiv \omega_f/(\omega_0) \ll 1, \]  

a much wider range of \( \omega_f \) will be considered afterwards.

Given that \( \omega_f \) is small, the system may be considered as moving in the quasi-stationary “wash-board” potential \( U \) with slope \( h\omega_0^2 \sin(\omega_ft) \). The absolute value of the slope is \( \sim h\omega_0^2 \) for most of the time while its sign is positive during odd half-periods of the perturbation, changing to the opposite one in the even half-periods. If the system is initially at the top of the potential barrier, then, owing to the condition (2), even a small slope
\[ \sim \hbar \omega_0^2 \text{ is sufficient to accelerate it during the first half-period up to a negative velocity of large absolute value.} \]

In the second half-period, the slope changes its sign, resulting in a braking effect, so that the velocity returns close to zero at the end of the period. Assuming that the maximum of the kinetic energy \( K \equiv p_f^2/2 \) greatly exceeds the spatial modulation of \( U(q,t) \),

\[ K_{\text{max}} \gg \omega_0^2, \quad (3) \]

one may neglect the term \( U_0(q) \) in \( U(q,t) \) while describing the major part of the trajectory (namely, when \( K \gg \omega_0^2 \)) during the first period of perturbation: the equations of motion reduce to those of a free particle driven by the time-periodic force, which are solved exactly:

\[ q(t) = A + \left( B - \frac{\hbar \omega_0^2}{\omega_f}\right) t + \frac{\hbar \omega_0^2}{\omega_f^2} \sin(\omega_f t), \]

\[ p(t) \equiv \dot{q} = B - \frac{\hbar \omega_0^2}{\omega_f^2} (1 - \cos(\omega_f t)), \quad (4) \]

where \( A = q(0) \) and \( B = p(0) \).

For the given initial state \((p(0) = 0, q(0) = \pi)\), \( B = 0 \) so that the velocity \((4)\) oscillates from 0 to \(-2\hbar \omega_0^2/\omega_f\) while the kinetic energy \( K \equiv p^2/2 \) oscillates from 0 to

\[ K_{\text{max}} = 2\hbar^2 \omega_0^2/\omega_f^2 \approx 2\hbar^2 \epsilon^2, \quad \epsilon \ll 1. \quad (5) \]

Eq. \((5)\) confirms the validity of the assumption \((3)\), and the maximum of the energy does diverge as \( \omega_f \to 0 \).

But Eqs. \((4),(5)\) do not explain chaos in the system. Like in other cases \(1, 2, 3, 4, 10\), the chaos onset in our system is related to the motion near the unperturbed separatix. Its rigorous treatment is complicated (cf. the conventional adiabatic case \(16\)) but is not essential for the quantity of main interest in our paper, i.e. for the chaotic layer width: the width is determined mainly by the “regular” parts of the chaotic trajectory (described by \((4)\)). So, we describe the chaos onset just qualitatively.

Define \( h_n \equiv h_n(\omega_f) \) as the value of \( h \) for which the system starting from the top of the barrier \((p(0) = 0, q(0) = \pi)\) arrives in the end of the first period of the perturbation \( t^{(1)} \equiv 2\pi/\omega_f \) at the top of the \( nth \) barrier i.e. \( \dot{q}(t^{(1)}) = 0, q(t^{(1)}) = \pi - 2n\pi \) where \( n \) is a large positive integer. If \( h = h_n \), the velocity of the system at the instant when it passed the previous (i.e. \((n - 1)st\)) barrier top can be shown to be \(-\dot{q}_c \) with \( \dot{q}_c \sim \sqrt{\hbar \omega_f \omega_0} \ln(\omega_0/(\hbar \omega_f)) \ll \omega_0 \).

Consider \( h \) slightly smaller than \( h_n \). For any \( t \), \(-\dot{q}(t)\) on the regular part of the trajectory is slightly smaller than that for \( h = h_n \). Hence, the velocity on the true trajectory becomes zero slightly to the right of the \( nth \) barrier top slightly before \( t^{(1)} \) i.e. the trajectory reflects from the right slope of the \( nth \) barrier and \( \dot{q}(t^{(1)}) > 0 \).

The new round of acceleration to the left starts only after the next reflection (from the left slope of the \((n - 1)st\) barrier) i.e. with a small delay \( \Delta t_f \) with respect to \( t^{(1)} \):

\[ \Delta t_f \sim \omega_0^{-1} \ln(\omega_0^2/\dot{q}_c^2) \sim \omega_0^{-1} \ln(\omega_0/(\hbar \omega_f)) \ll \omega_f^{-1}. \quad (6) \]

This new round of acceleration-braking is described by Eq. \((4)\) with \( B \) determined by the condition \( p(2\pi/\omega_f + \Delta t_f) = 0 \), i.e. \( B = (\omega_0/\epsilon)(1 - \cos(\omega_f \Delta t_f)) \geq 0 \).

Consider \( h \) slightly larger than \( h_n \). For any \( t \), \(-\dot{q}(t)\) is slightly larger than that for \( h = h_n \) on the regular part of the trajectory. Hence, at \( t^{(1)} \), the system arrives slightly to the left of the top of the \( nth \) barrier while moving to the left and with an energy close to the top of the barrier level. When the coordinate of the system approaches the vicinity of the top of the next (i.e. \((n + 1)st\)) barrier of \( U(q,t) \), the latter becomes sufficiently lower than the top of the \( nth \) barrier and the system passes over it rather than reflects. Thus, the second round of acceleration-braking is described by Eq. \((4)\) with \( B \equiv \dot{q}(t^{(1)}) \) being negative with a small absolute value.

At the end of the second acceleration-braking round, the system may again either pass over a barrier or reflect from it and even pass in the backward direction for a few periods of the potential. In the latter case, the new acceleration-braking round is additionally delayed with respect to the perturbation by some time \( \Delta t_f \): this round is described by \((4)\) with yet a larger positive \( B = (\omega_0/\epsilon)(1 - \cos(\omega_f (\Delta t_f + \Delta t_{(2)}))) \geq 0 \). As time goes on, the process of reflection develops and, on long time-scales, the delay due to the reflections is accumulated. So, \( B \) gradually grows in average until it gets close to \( B_{\text{max}} \equiv 2\omega_0/\epsilon \), then gradually decreases in average until it gets close to 0, etc. The sequence of reflections/passings is random unless \( h = h_n \), but even in this case the sequence is random if the initial state is shifted from the top of the barrier. As reflections/passings and intervals \( \Delta t_f \) are random, variations of \( B \) are random too: so, the trajectory is chaotic on large time-scales.

Note also that the action \( I \equiv \int (2\pi)^{-1} \psi^2 dq \), conventionally \(4, 10, 11\) chosen as the lowest-order adiabatic invariant, is not conserved for motion above the barrier in our system: on the major part of a trajectory, \( K \gg \omega_0^2 \) and hence \( I \equiv p \) while \(|p| \) varies in a wide range (from 0 to \( \sim \omega_0/\epsilon \), for the chaotic trajectory). The correct lowest-order adiabatic invariant for our system is

\[ I = I + \frac{\hbar \omega_0^2}{\omega_f} (1 - \cos(\omega_f t)). \quad (7) \]

To the lowest order in \( \epsilon \), \( I \) coincides with the integration constant \( B \) of \((4)\) on the major part of the trajectory \(17\). So, the chaotic layer width in \( I \) is the same as in \( B \), i.e. equal to \( B_{\text{max}} \equiv 2\hbar \omega_0^2/\omega_f \), diverging as \( \omega_f \to 0 \).

Let us consider the problem of the layer width in a more general case, when Eq. \((2)\) may not be satisfied. As explained above, the trajectory that can both pass over a barrier and reflect from it is chaotic. But the strong
inequality (3) for $K_{max}$ may not hold now (cf. Eq. (5)) so the term $U_0$ in $U$ cannot be neglected even on regular parts of the chaotic trajectory. Let the adiabatic approximation be still valid (the explicit condition is derived in Eq. (18)). As $h$ is small, the turning point of the chaotic trajectory is situated near the top of a potential barrier:

$$p(t_s) = 0, \quad q(t_s) \approx \pi - 2\pi m,$$

where $m$ is integer and $t_s$ is one of instants when $p = 0$.

Let $K_n$ be the kinetic energy $K$ at the instant $t_n$ when the system crosses the coordinate of the top of the $n$th barrier of the auxiliary potential $U$, i.e.

$$q(t_n) = q_n \approx \pi - 2\pi n, \quad K_n = \frac{p^2(t_n)}{2}.$$  \hspace{1cm} (9)

The coordinate of the next barrier top crossed by the system is

$$q_{n+\delta_n} \approx q_n - 2\pi \delta_n, \quad \delta_n \equiv -\text{sign}(p(t_n)).$$  \hspace{1cm} (10)

In the adiabatic approximation, the change of $K$ during the time $t_{n+\delta_n} - t_n$ is the following:

$$K_{n+\delta_n} - K_n \approx -(q_{n+\delta_n} - q_n)\hbar^2\sin(\omega t_n).$$  \hspace{1cm} (11)

The interval of time $t_{n+\delta_n} - t_n$ can be evaluated in the adiabatic approximation as follows

$$t_{n+\delta_n} - t_n \equiv \int_{q_n}^{q_{n+\delta_n}} \frac{dq}{p} \approx 2\sqrt{2K(x)} \frac{\pi}{\omega_0},$$

$$K(x) \equiv \int_{0}^{\frac{\pi}{2}} \frac{d\varphi}{\sqrt{1 - x \sin^2(\varphi)}}, \quad x \equiv \frac{1}{1 + \frac{K}{(2\omega_0^2)}}.$$ 

$K(x)$ is the full elliptic integral of the 1st order [18].

Significant changes of $K_n$ take place on the time scale $\omega_f^{-1}$ while the adiabatic condition means that

$$t_{n+\delta_n} - t_n \ll \omega_f^{-1}.$$  \hspace{1cm} (13)

So, discrete changes of $K_n \equiv K(t_n)$ may be replaced by the continuous change of a function $\dot{K}(t_n)$ with derivative

$$\frac{d\dot{K}}{dt_n} \approx \frac{K_{n+\delta_n} - K_n}{t_{n+\delta_n} - t_n} \approx -\text{sign}(p(t_n)) \frac{\pi \hbar^3 \sqrt{1 + K/(2\omega_0^2)}}{K(1/(1 + K/(2\omega_0^2)))} \sin(\omega f t_n).$$  \hspace{1cm} (14)

Separating variables, evaluating the resulting integrals and taking into account that, within the present simplified description of motion, $\text{sign}(p)$ changes when $K = 0$, we obtain the transcendental equation for $\dot{K}$:

$$E(x) \frac{\sqrt{x}}{\sqrt{1 - x^2}} = 1 + \frac{\pi \hbar \omega_0}{4 \omega_f} \cos(\omega_f t_n) - \cos(\omega_f t_n),$$  \hspace{1cm} (15)

$$E(x) = \int_{0}^{\frac{\pi}{2}} d\varphi \sqrt{1 - \sin^2(\varphi)}, \quad x \equiv \left(1 + \frac{\dot{K}}{2\omega_0^2}\right)^{-1}.$$  \hspace{1cm} (16)

Here, $E(x)$ is a full elliptic integral of the 2nd order [18].

Due to the random-like changes of $t_s$, $\cos(\omega_f t_s)$ on long time-scales is densely distributed over the range $[-1,1]$. Maximizing $\dot{K}$ with respect to $t_s$ and $t_n$ and taking into account that $E(t_n) = K(t_n) + U_0(q(t_n)) \approx K(t_n) + \omega_0^2$, we finally obtain the transcendental equation for the upper energy boundary of the chaotic layer $E_{max}$:

$$E(x) \frac{\sqrt{x}}{\sqrt{1 - x^2}} = 1 + \frac{\pi \hbar \omega_0}{2 \omega_f}, \quad x \equiv \left(1 + \frac{E_{max} - \omega_0^2}{2\omega_0^2}\right)^{-1}.$$  \hspace{1cm} (17)

$E_{max}$ monotonously decreases from $\infty$ to $\omega_0^2$ as $\omega_f/\hbar \omega_0 \equiv \epsilon$ increases from 0 to $\infty$. Fig. 2 shows that Eq. (16) nicely describes the simulations in a wide range of $\omega_f$.

![FIG. 2: Spectral dependence of the maximum energy in the chaotic layer ($\omega_0 = 1, h = 0.01$): circles, solid, dashed and dotted lines correspond respectively to simulations, the general formula (16), the asymptotes (5) and (17).](image)

For $\epsilon \ll 1$, the root $(E_{max} - \omega_0^2)/\omega_0^2$ of Eq. (16) is large. So, $x \approx 2\omega_0^2/E_{max} \to 0$ while $E(x \to 0) \to \pi/2$, and the solution of (16) reduces to the asymptote (5).

For $\epsilon > 1$, the root $(E_{max} - \omega_0^2)/\omega_0^2$ of Eq. (16) is small. Using the asymptote [18] for $E(x \to 1)$, Eq. (16) can be reduced to the following asymptote for $E_{max}$:

$$\frac{E_{max} - \omega_0^2}{\omega_0^2} \approx \frac{32}{a \ln(a)}, \quad a \equiv \frac{8\epsilon}{\pi}, \quad \epsilon \gg 1.$$  \hspace{1cm} (18)

Using the estimate (12) and the asymptote $K(x \to 1) = 0.5 \ln(16/(1-x))$ [18] and allowing for Eq. (17), we may express the adiabatic condition (13) explicitly:

$$\omega_f \ll \omega_0/\ln(1/h).$$  \hspace{1cm} (19)

Let us discuss chaotic transport. For most physical applications, transport in coordinate is relevant. For sufficiently long time-scales, the chaotic trajectory provides large-scale displacements in both directions, unlike regular trajectories. Generally, the mean-square displacement for chaotic transport depends on time as $t^{3/2}$.
\( \langle q(t) - q(0) \rangle^2 = D t^b \) with \( 0 < b < 2 \) (\( \langle \ldots \rangle \) means averaging of the initial conditions over the chaotic layer). The larger \( D \) and \( b \) are, the faster the transport is. It is suggested in [19], basing on numerical results, that \( b \to 1 \) as \( \omega_f \to 0 \). As for \( D \), we suggest that it strongly diverges. Indeed, chaotic trajectories generally spend most of the time close to the boundaries of regions of regular motion [25]. In our case, it means that, for most of the time, the trajectory moves close to either the upper border of the chaotic layer, with the average velocity \( v \approx h \omega^2_0/\omega_f \), or the lower border, with the average velocity \(-v\). We call such regimes acceleration-braking flights (cf. [20]), distinguishing them from the regime of diffusion across the layer. The duration \( t_f \) of the flight may be estimated from the analysis of the diffusion of \( B \) near the boundary of the layer. The diffusion constant for \( B \) may be roughly estimated as \( D_B \sim \langle (\Delta B)^2 \rangle / (2\pi/\omega_f) \) where \( \langle (\Delta B)^2 \rangle \) is the average squared change of \( B \) at the end of a driving period: \( \langle (\Delta B)^2 \rangle \sim B_{max}^2 (\omega_f / D t_f)^4 \). Then,

\[
t_f \sim \frac{B_{max}^2}{D_B} \sim \omega_0^{-1} \left( \frac{\omega_0}{\omega_f} \right)^5 \ln^2 \left( \frac{\omega_0}{(h \omega_f)} \right).
\]

Finally, \( D \) may be estimated as the ratio between the squared length of the flight \( l_f^2 \) and its duration \( t_f \):

\[
D \sim \frac{l_f^2}{t_f} = v^2 t_f \sim \omega_0 h^2 \left( \frac{\omega_0}{\omega_f} \right)^7 \ln^2 \left( \frac{\omega_0}{(h \omega_f)} \right).
\]

The above analysis provides intuitive arguments in favor of a strong acceleration of the chaotic transport in space as \( \omega_f \to 0 \), and simulations support this. Still, a thorough numerical study and a rigorous evaluation of \( D(\omega_f) \) as well as a proof that \( b(\omega_f \to 0) = 1 \) are necessary.

Apart from purely dynamic phenomena, our work may have a strong impact on noise-induced phenomena: e.g. diffusion of particles on surfaces (see [18] and references therein), that plays an important role in many modern technologies involving self-assembled molecular-film growth, catalysis, and surface-bound nanostructures [21]. Numerous studies of atoms (e.g. [22]), organic molecules (e.g. [23]), and even metal clusters (e.g. [24]) show that the long jumps may play a dominant role in the diffusion: this means that the damping is small. If we add a weak ac drive, then transient chaos [2] arises in a region of phase space which approximately coincides with the chaotic layer developed for zero damping (cf. [1]). In the light of the present results, the latter means: if the driving is adiabatic, then, as soon as the noise activates the particle to the lower boundary of the layer (i.e. approximately to the barrier level), the further transport is provided by fast (compared to slow noise-induced diffusion) chaotic transport. Thus, even a weak drive may drastically increase the speed of the diffusion.

One more possible application concerns a threshold device (cf. [25]). If the device was based on a noise-driven spatially periodic system and switched at the energy level \( E_{th} \) significantly exceeding the barrier level \( U_b \), then the addition of even a weak but sufficiently slow ac drive would give rise to a marked decrease of the activation energy - from \( E_{th} \) to \( U_b \), thus leading to a drastic increase of the flux. This may also be used as a sensitive method to measure the amplitude/frequency of the drive.

In conclusion, we have discovered the divergence of the chaotic layer width and the related strong acceleration of the chaotic spatial transport in ac driven periodic systems in the adiabatic limit. The mechanism is a combination of acceleration-braking flights of high average kinetic energy and of small random changes of the adiabatic invariant near the separatrix. Applications to diffusion on surface and to threshold devices have been suggested.

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1. See [18], [20, 21] for references.