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Escape Rates in Hamiltonian Systems

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Particles escape from the vicinity of invariant tori is macroscopically modeled by a nonuniform diffusive process. The space dependence of transport coefficients is fixed by using perturbation theory scalings. This leads to universal predictions for the escape rates that are then observed in numerical simulations.

KEY WORDS: Invariant tori; normal forms; resonances; transport; diffusion; escape rates.

I. INTRODUCTION

Dynamical astronomers have started in the latest years quantitative investigations of long-time effects in the Solar System. The progresses in computational methods permit now to follow the evolution of thousands of test particles over times of the order of billions of years. A specific attention has been paid to the rates which characterize the escape of particles from the asteroid and the Kuiper belt.[1-4] A striking result of numerical studies is that specific laws for the escape rates seem to universally appear for particles initially located in the vicinity of some stable resonant islands.[4] This observation motivated us to investigate in general terms the possible connections between escape rates and the dynamical structures ruling diffusion processes in Hamiltonian systems.

It is known that a crucial role in structuring diffusion is played by invariant KAM tori, either in the form of rotational curves or of resonant islands. Particles initially located far from tori escape very rapidly on account of the strong chaoticity of these regions. The behaviour at large enough times of the escape rates is therefore dominated by particles with initial conditions in the close neighbourhood of invariant tori. These are the orbits on which we shall concentrate our attention here. Particles

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nearby the torus escape slower and slower as the distance d from the torus decreases. Perturbation theory provides the scaling lows with d of the size of the effective perturbation, which is responsible for the actions changes.

In addition to invariant tori, also cantori can structure diffusion processes. Their global effect is somehow similar to a hardly permeable barrier. However, this effect is generically relevant only in systems with two degrees of freedom. Their spatial extension is indeed very minute. It is therefore reasonable to expect that, in systems with more than two degrees of freedom, the particles are statistically able to efficiently go round them. The dominant effect is then the dependence of actions variations on the distance from the torus and we can macroscopically model particles escape as a non-homogeneous diffuse process. The space-dependence of transport coefficients is fixed by using perturbation theory scalings, discussed in Section 2. This permits us to derive the long-time dominant behaviour of the escape rates for a general class of normal forms which are valid in the vicinity of an invariant torus. In particular, Kolmogorov quadratic normal form and Nekhoroshev exponential normal form are shown to lead to $t^{-3/2}$ and $1/t \log^a t$ escape rates (with some positive a depending on the number of degrees of freedom). In systems with two degrees of freedom these laws are cut-off at very large times by the barrier effects due to cantori. Their low permeability leads to a sporadic Poissonian regime characterized by an exponential decay of the escape rate. The predicted laws are tested on well known 2D and 4D model maps in Section 3, where we also discuss other numerical results in the existing literature.

2. NORMAL FORMS AND ESCAPE RATES CLOSE TO INVARIANT TORI

The results provided by perturbation theory concerning the size of the remainder of normal forms are commonly believed to be just upper bounds. The scaling behaviours they provide seem then to have no specific physical meaning. However, this is not the case: the optimal remainder of normal forms has indeed a direct physical meaning since it is intimately related to the size of the effective resonant perturbation of the system. This result has been recently obtained in ref. 5 and we shall here briefly recall the basic ideas. Let us fix the domain where the convergence of the normal form is required. Without any loss of generality, the Hamiltonian of the system can be split as

$$H(p, q) = h_{\mathrm{norm}} + h_{\mathrm{res}} + h_{\mathrm{nonres}}, \tag{1}$$

where h_{norm} is in normal form and the remainder is split in two parts: h_{res} containing only Fourier modes corresponding to resonances inside the considered domain and h_{nonres} with all the other terms. The terms in h_{nonres} can be eliminated by canonical transformations. In this process of elimination, resonant terms will generically appear, even if initially absent, and cannot be subsequently reduced without shrinking the domain of convergence. The best normal form is therefore the one where all non-resonant terms have been reduced to be negligible with respect to h_{res}. As a consequence, h_{res} fixes the size of the remainder of the optimal normal form. Simple considerations on the order of the resonances crossing the domain allow then to predict the "generic" size of h_{res}.

With these considerations in mind, we now proceed to discuss the scaling of the remainders in the vicinity of an invariant torus. These scalings will then be used in Section 2.2 for the modelization of the escape process.

2.1 Normal Forms

Let us consider a Hamiltonian dynamical system with an invariant torus that, without loosing any generality, can be assumed to be in $p = 0$. Following Kolmogorov[6], it is possible to transform the Hamiltonian to the *local* quadratic normal form

$$H(p, q) = \omega \cdot p + \mathscr{R}(p, q) \qquad \text{with} \quad \mathscr{R} = O(|p|^2), \tag{2}$$

which is analytic up to some threshold distance d_1 from the invariant torus. This is evidently the minimal normal form compatible with the existence of an invariant torus carrying linear flow in $p = 0$. Our aim now is to get the optimal normal forms, in the sense previously discussed. Following again ref. 5, let us split $\mathscr{R}$ in h_{res} and h_{nonres}, where h_{nonres} contains all the non-resonant terms in a neighbourhood of radius d of $p = 0$. The h_{nonres} can be eliminated by canonical transformations. The size of the optimal remainder h_{res} depends on d. Kolmogorov normal form is optimal when the distance d from the torus satisfies $d_2 < d < d_1$, for some threshold d_2. For $d < d_2$, the resonant part h_{res} becomes significantly smaller than $\mathscr{R}$ in (2). It is indeed simple to show that h_{res} contains only harmonics of Fourier order larger than $1/d^{\alpha}$, where α is a positive parameter depending on the number of degrees of freedom and the properties of the frequencies ω of the invariant torus. For analytic Hamiltonians the Fourier modes will asymptotically decrease exponentially with respect to their order. It follows that h_{res}

decreases exponentially in $1/d^\alpha$. This shows that in the domain $|p| < d_2$ the optimal normal form is

$$H(p, q) = \omega \cdot p + \mathscr{B}(p) + \mathscr{R}'(p, q) \qquad \text{with} \quad \mathscr{R}' = O(\exp[-1/|p|^\alpha]), \tag{3}$$

where $\mathscr{B}(p)$ depends only on the action variables. Due to the exponential dependence of $\mathscr{R}'$ on d, we will refer to (3) as the *Nekhoroshev normal form*, in the neighbourhood of a KAM torus.

We now proceed to discuss the dynamical structure of the Hamiltonian system (3). Since the size of the effective perturbation $\mathscr{R}'$ decreases exponentially with the inverse of the distance from the torus, there must be a third threshold $d_3 < d_2$ such that for $|p| < d_3$ the perturbation $\mathscr{R}$ is small enough to allow the application of Nekhoroshev theorem.[7] As discussed in ref. 8 (see also ref. 9), the possibility of application of Nekhoroshev theorem implies a basic change of the dynamical structure of the system. When the Nekhoroshev theorem cannot be applied, there is no place for invariant tori inside the meshes of the Arnold web. Diffusion and transport phenomena should be dominated by resonance overlapping. As a consequence, we expect that the change of actions is proportional to the size of the effective perturbation of the system. Conversely, when the Nekhoroshev theorem can be applied, resonances cannot overlap, in the sense that invariant tori fill a large volume of each mesh of the Arnold web. In this situation, the dominant mechanism of diffusion should be the one described by Arnold,[10] usually known as "Arnold diffusion". The estimates provided by Nekhoroshev show that the transport times are at least exponentially long with respect to the inverse of the effective perturbation. Since the perturbation $\mathscr{R}'$ is $O(\exp[-1/|p|^\alpha])$, then the escape times must be longer than $O(\exp[\exp[1/|p|^\alpha]])$, namely they increase superexponentially with the inverse of the distance from the torus at $p = 0$.

2.2 Escape Rates

The conclusion arising from the results illustrated in Section 2.1 is that the dominant *microscopic* mechanism of escape from the region $d_3 < |p| < d_1$ is the overlapping of resonances. The amplitude of the latter is governed by the scaling laws of the effective perturbation. The escape process involves *macroscopic* time scales, i.e., much larger than those associated with the crossing of a single resonance. The other crucial point for the escape process is the existence of a gradient of the effective perturbation in the direction outwards the torus. These two remarks lead us to model the escape process by a nonuniform diffusion with transport coefficients scaling according to (2) and (3).

Specifically, let us consider the unit interval $I = [0, 1]$. A very large number of particles is initially uniformly distributed on I. The position $x(t)$ of a particle evolves according to the following equation

$$\frac{dx(t)}{dt} = s(x)\, b(t), \tag{4}$$

where $b(t)$ is the usual Gaussian noise having zero average and white-in-time:

$$\langle b(t), b(t') \rangle = 2D\delta(t - t'). \tag{5}$$

The noise $b(t)$ should be thought as the limiting case of colored noise with correlation-time tending to zero. The multiplicative noise term in (4) is therefore to be interpreted in the Stratonovich sense.[11]

For $s(x) = \text{const}$, Eq. (4) is the usual Langevin equation corresponding to an ordinary diffusive process. The function $s(x)$ is intended to represent the dependence of the size of the effective perturbation on the distance from the torus. For a Kolmogorov normal form (2), we would for example consider $s(x) = x^2$, while for Nekhoroshev normal form (3): $s(x) = \exp(-1/x^\alpha)$. More generally, we shall consider the following two classes:

$$\begin{aligned} &\text{(a)} \quad s(x) = x^\beta \quad \text{with} \quad \beta > 1; \\ &\text{(b)} \quad s(x) = \exp(-1/x^\alpha) \quad \alpha > 0. \end{aligned} \tag{6}$$

The regions far away from the torus are strongly chaotic and particles getting there are essentially lost. We thus impose absorbing boundary conditions at $x = 1$ and calculate the escape rate as the current $J(t)$ flowing out of I at the boundary $x = 1$.

The key for the analytical solution of the problem is the definition of the new variable

$$y(x) = \int_x^1 \frac{dz}{s(z)}. \tag{7}$$

The equation for $y(t)$ reduces indeed to

$$\frac{dy(t)}{dt} = b(t), \tag{8}$$

where the $-$ sign has been omitted because b and $-b$ are statistically equivalent. The point $x = 1$ corresponds to $y = 0$, while $x = 0$ is mapped at infinity. We are thus left with an ordinary diffsive process on the positive half-line, with absorbing boundary condition at the origin. The initial distribution of particles $P(y, 0)$ on the half-line is immediately obtained from the definition (7):

$$P(y, 0) = |dx/dy|\, P(x, 0) = |dx/dy| = s(x(y)) \equiv \tilde{s}(y). \tag{9}$$

The rate of escape $J(t)$ is simply given by (see, e.g., ref. 12)

$$J(t) = D(\nabla_y P)(0, t), \tag{10}$$

where the derivative has to be evaluated at $y = 0$.

The evolution of the probability distribution $P(y, t)$ is obtained by using the classical diffusive Green function with absorbing boundary condition:[12]

$$P(y, t) = \int_0^\infty P(z, 0) \frac{1}{\sqrt{4\pi Dt}} \left[\left(\exp - \frac{(y-z)^2}{4Dt} \right) - \left(\exp - \frac{(y+z)^2}{4Dt} \right) \right] dz. \tag{11}$$

It follows from (10) and (11):

$$\begin{aligned} J(t) &= D \int_0^\infty \frac{\tilde{s}(z)}{2\sqrt{\pi Dt}\, Dt}\, z \exp\left(-\frac{z^2}{4Dt} \right) dz \\ &= \sqrt{\frac{D}{\pi t}} \int_0^\infty \tilde{s}(\sqrt{4Dtz}) \exp(-z)\, dz. \end{aligned} \tag{12}$$

Let us now specify (12) to the two classes (6). For (a), the inversion in (7) is easily performed and gives

$$\tilde{s}(y) = (1 + (\beta - 1) y)^{\beta/(1-\beta)} \tag{13}$$

Inserting this expression into (12) we obtain the large-time behaviour of the escape rate

$$J(t) \simeq t^{-(2\beta - 1)/(2\beta - 2)}. \tag{14}$$

For class (b) the inversion of (7) is not immediate. However, for the large-time escape rate it is relevant just the behaviour of $\tilde{s}$ for large values of the argument. The dominant term of the asymptotic expansion of (7) is

$$y(x) = \left(\frac{1}{\alpha} x^{1+\alpha} + O(x^{1+2\alpha}) \right) \exp\left(\frac{1}{x^\alpha} \right).$$

The resulting expression of the function $\tilde{s}(y)$ defined in (9) is

$$\tilde{s}(y) \simeq (y(\log y)^{1+1/\alpha})^{-1}. \tag{16}$$

Inserting (16) into (12) it follows that the escape rate for large times is:

$$J(t) \simeq (t(\log t)^{1+1/\alpha})^{-1}. \tag{17}$$

Note that, except for logarithmic corrections, (17) is the limit of (14) for $\beta \to \infty$.

3. NUMERICAL EXPERIMENTS

In order to test the validity of the model presented in the previous section, we perform now a few numerical experiments on simple symplectic maps. We focus in particular on regions in the neighbourhood of invariant tori, uniformly distribute a large number of particles and measure their rate of escape as a function of time.

Let us first consider the usual standard map

$$q' = q + p, \qquad p' = p + K \sin q',$$

with $K = 0.12$. For this value of the parameter, it is known that the chaotic region associated to the main resonance at $p = 0$ is bounded by invariant tori. We distributed 10^5 particles in the box $q \in [-0.0002, 0.0002]$, $p \in [-0.0002, -0.0001]$, which is crossed by the boundering torus. Previous numerical experiments showed that this region is very sticky[15] and is thus appropriate for our purposes. More precisely, it is observed that when the particles get out of the sticky region close to the boundary torus, they quickly flow into the chaotic region associated to the main resonance. The action p then rapidly becomes positive. We thus define as "escaped" the particles evolved to $p > 0$. The histogram of the number of escapers (smoothed with a running average) *vs* the map iteration number is shown in Fig. 1a in log–log scale. Around $10^{5.5}$ iterations, the escape rate varies with time approximately as a power law with exponent close to $-3/2$; the slope then decreases and finally there is a sharp fall off. The latter turns out to be exponential as revealed by the lin–log plot in Fig. 1b, i.e., the rate of decrease of the remaining particles N is $dN/dt \sim \exp(-t/\tau)$. The exponential fall off is due to the presence of a cantorus close to the bounding torus.

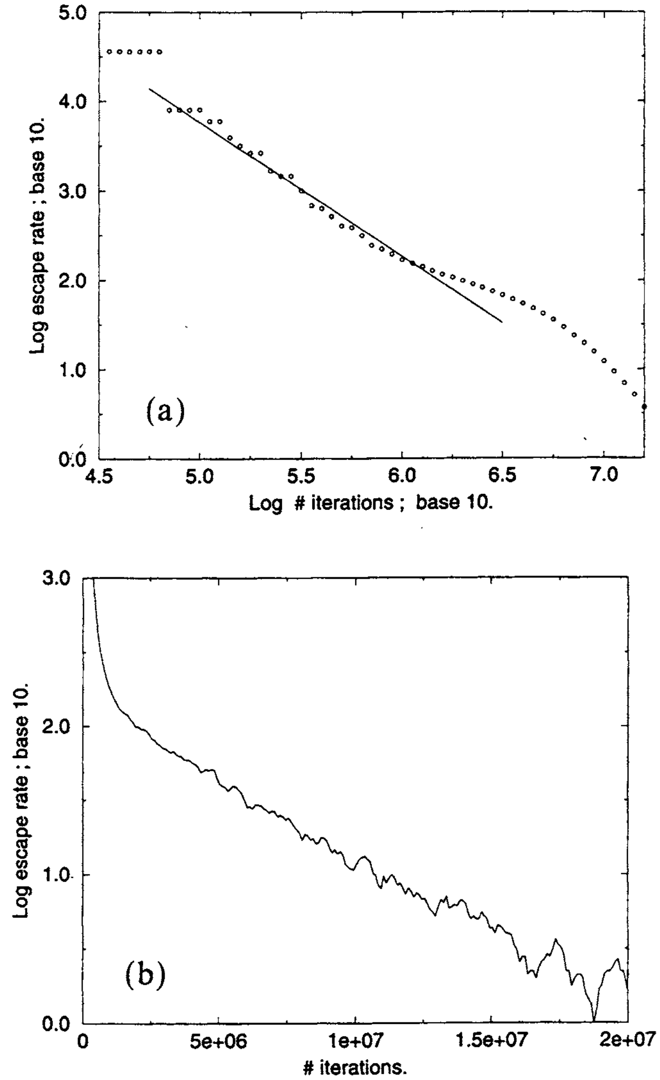

Fig. 1. The escape rate vs. the number of iterations in Standard Map's experiment. In panel (a) (on the left), a reference line with slope $-3/2$ is plotted.

The key property of such cantorus is to have very small gaps. The typical time τ for crossing is therefore very large. On the other hand, the particles initially located between the torus and the cantorus have to cross the latter to escape. Since τ is very large, the particles behind the cantorus have time to get mixed and their probability to find a gap is very low. The conditions for a Poissonian régime[13] are therefore satisfied and the average number of particles escaping in the unit time is proportional to N/τ, as in classical radioactive decay processes. We have checked this behaviour looking at the original position of the escapers as a function of the escape time. For times in the exponential regime the escapers are initially located between the torus and the cantorus and the escape times are completely mixed. On the contrary, for smaller times, the escapers are initially located beyond the cantorus and we observe a smooth gradient of the escape times with their distance from the bounding torus. On the basis of this argument, one expects that the exponential behaviour does not last foreover. Indeed, sufficiently close to the invariant torus, the characteristic times should become larger than τ, so that particles would not have enough time to get mixed. Our numerical experiment shows that in 2D maps the exponential behaviour, although possibly transient and not universal, can be the dominating one over huge timespans.

The barrier effect of the cantorus should disappear if the number of degrees of freedom is increased. We have therefore considered the 4D Hénon map studied in ref. 14, which is equivalent to a Hamiltonian dynamical system with three degrees of freedom. In ref. 14 the authors found that there is a very stable core around the center of the map $p_1 = p_2 = 0$, where invariant KAM tori fill most of the volume. Moreover, they found a gradient of escape times along the radial direction. Far from the center the particles escape very rapidly, while the escape times increase sharply approaching the central stable core. The authors of ref. 14 have uniformly distributed 10^5 particles in a box in the action space bounding the stable core and defined as "escaped" the particles getting out of the box. Using their data, kindly provided to us, we have plotted in Fig. 2 the histogram of the number of escapers *vs* the map iteration number. No exponential fall off is observed, as expected.

A neat $t^{-3/2}$ scaling is observed, followed by a slow decrease of the slope. The slope $-3/2$ is in agreement with (14) for $\beta = 2$, corresponding to Kolmogorov normal form (2). The dashed line has slope -1, corresponding to the asymptotic expression of (17). The last part of the data seems to approach such a slope, even though the transition looks very gradual. This can be understood as follows: the transition from Kolmogorov to Nekhoroshev normal form is realized through a sequence of Birkoff normal forms of increasing polinomial order β. The Nekhoroshev exponential normal form is the asymptotic fit of such sequence. For each of the polynomial normal forms, formula (14) holds. Therefore formula (17) should be interpreted as the asymptotic expression of (14) for $\beta \to \infty$.

A further test of the predicted escape rate laws is provided by Fig. 3, which refers to a 4D Henon map with corrections of eighth polar order

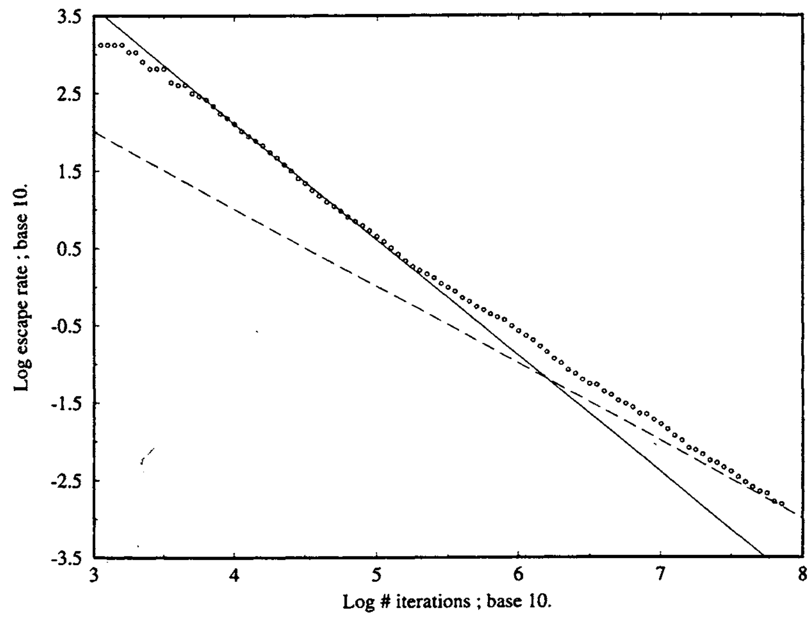

Fig. 2. The escape rate vs. the number of iterations in 4D Henon Map's experiment. Reference line with slope $-3/2$ (solid) and -1 (dashed) are plotted.

(see ref. 14). Again, we observe a decrease of the escape rate with slope $-3/2$, followed by a slow relaxation to the asymptotic slope -1.

Alternative studies on the escape of particles located close to invariant tori in systems with more than two degrees of freedom can be found in refs. 15 and 16. The existence of a region ruled by Kolmogorov quadratic normal form is neglected. The escapes are assumed to happen *via* a ballistic motion

$$\frac{dx(t)}{dt} = s(x), \tag{18}$$

where $s(x)$ is given by (b) in (6), according to Nekhoroshev law. The escape rate of this process coincides at the leading order with our formula (17). Note that this coincidence at the dominant order is due to the specific form of $s(x)$ and would not be true, for example, for the normal forms of class (a) in (6). To check their predictions in numerical simulations, the authors do not compute directly the escape rate: they measure respectively

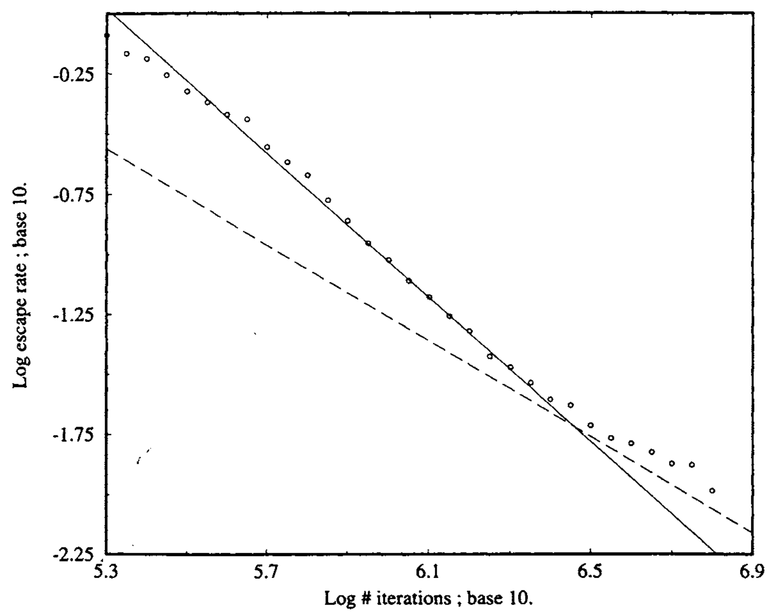

Fig. 3. The same as Fig. 2 but for the 4D Henong Map with eight polar order corrections.

in ref. 16 the number of remaining particles as a function of time, and in ref. 15 the escape times as a function of the initial coordinates. This involves some free parameters which are fixed by fitting the numerical data.

4. CONCLUSIONS

We have shown that modelling the escape process of particles in the neighbourhood of invariant tori by a non-uniform diffusion leads to well-defined universal predictions for the escape rates. In 2D systems the barrier effects due to cantori can lead to a peculiar exponential fall-off at very large, but finite, times. The predicted rates of escape have been observed in numerical simulations of 2D and 4D symplectic maps.

This makes us confident that measuring the escape rates can be a useful numerical tool to explore the structure of dynamical systems with many degrees of freedom. In particular, a $-3/2$ power law behaviour followed by a slow decrease of the slope to the asymptotic value -1 can be considered as a strong indication of the existence of invariant tori. Particles escape is then eroding their close neighbourhood characterized by a Kolmogorov and a Nekhoroshev normal form, respectively.

From a theoretical point of view, our results point to the *macroscopic* picture of the escape dynamics as a stochastic motion *microscopically* induced by resonance overlapping and driven away from the torus by the gradient of the effective perturbation.

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