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Observable and hidden singular features of large fluctuations in nonequilibrium systems

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Abstract

We study local features, and provide a topological insight into the global structure of the probability density distribution and of the pattern of the optimal paths for large rare fluctuations away from a stable state. In contrast to extremal paths in quantum mechanics, the optimal paths do *not* encounter caustics. We show how this occurs, and what, instead of caustics, are the experimentally observable singularities of the pattern. We reveal the possibility for a caustic and a switching line to start at a saddle point, and discuss the consequences.

The problem of large occasional fluctuations in nonequilibrium systems is of substantial general interest and importance. These fluctuations form the tails of statistical distribution, give rise to escape from a stable state, and are responsible for the onset of many effects investigated in various areas of physics – some recent examples are stochastic resonance [1] and transport in ratchets [2]. One of the basic concepts in the analysis of large fluctuations is optimal path – the path along which the system moves, with overwhelming probability, on its way to a given point remote from the stable state. Optimal paths are experimentally observable, and have been an object of active study for the last 20 years (see Refs. [3,4] for a review). They play, in the context of fluctuations, the same role as trajectories for dynamical systems,

and therefore understanding the pattern of the optimal paths is a key to understanding large fluctuations.

From the formal point of view, optimal paths are similar to the extremal paths in quantum mechanics since both provide an extremum to the integrands in the appropriate path integrals. A well-known feature of the pattern of the extremal paths is the occurrence of caustics [5]. Caustics have also been revealed numerically in the pattern of optimal paths for fluctuating systems of various types [6–11]. For quantum mechanical systems the physical meaning of caustics is well understood – a semiclassical wave function is oscillating on one side of a caustic and exponentially decaying (or increasing) on the other side. In contrast, the probability density distribution, which is determined by the optimal paths, is nonnegative definite. Therefore it cannot be continued beyond a caustic, and it follows that caustics may *not* be encountered by these paths.

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In the present paper we address the problem of avoidance of caustics by the physically meaningful optimal paths, and of the global structure and the observable singularities of the pattern of these paths. The physical and topological arguments we apply are quite general, but as an illustration of how they work we consider the simplest case, that of a two-variable system performing Brownian motion described by the stochastic equation

$$\dot{q}_i = K_i(q) + \xi_i(t), \quad q \equiv (q_1, q_2),$$

$$\langle \xi_i(t) \rangle = 0, \tag{1}$$

$$\langle \xi_i(t)\xi_j(t') \rangle = D\delta_{ij}\delta(t - t'), \quad i,j = 1,2.$$

Here, $\xi(t)$ is Gaussian white noise. The drift coefficients $K_{1,2}$ are assumed nonsingular for finite q.

We assume noise intensity D to be small. In this case if the system is prepared initially within the basin of attraction of an attractor a, it will most likely approach the attractor in a characteristic relaxation time t_{rel}, as if there was no noise. Then it will perform mostly small fluctuations about the position of the attractor q_a, so that over t_{rel} a (quasi)stationary probability density distribution $\rho_a(q)$ will be formed. Large fluctuations occasionally bring the system to points q remote from q_a, and thus form the tails of $\rho_a(q)$. To logarithmic accuracy [3]

$$\rho_a(q) = \text{const} \times \exp[-S_a(q)/D], \tag{2}$$

where $S_a(q)$ is given by the solution of the variational problem

$$S_a(q) = \min \int_{-\infty}^{0} \mathcal{L}(\dot{q}(t), q(t)) \, dt, \tag{3}$$

$$\mathcal{L}(\dot{q}, q) = \tfrac{1}{2}(\dot{q} - K)^2, \quad q(-\infty) = q_a, \quad q(0) = q.$$

Eq. (3) defines the optimal (most probable) path $q_{\text{opt}}(t)$ to a point q from the stable position q_a ($K(q_a) = 0$), in the small vicinity of which the large fluctuation starts. The optimal path can be associated with the trajectory of an auxiliary four-variable (two coordinates, $q_{1,2}$, and two conjugate momenta, $p_{1,2}$) Hamiltonian system, with the action $S_a(q)$ and Lagrangian $\mathcal{L}$ (3), and with the respective Hamiltonian $\mathcal{H} = \tfrac{1}{2}p^2 + p \cdot K$. The Hamiltonian equations of motion for the trajectories are of the form

$$\dot{q} = K + p, \quad \dot{p} = -(p \cdot \nabla)K - p \times (\nabla \times K), \tag{4}$$

where these trajectories lie on the energy surface $E = 0$.

The approximation (2) is similar to the WKB approximation in quantum mechanics, with the noise intensity D corresponding to $i\hbar$. As in quantum mechanics, the extremal paths $q(t)$ (3), (4) intersect each other, generically, and the set of these paths displays caustics [6–8].

An interesting example of a system where caustics occur [9] is an underdamped nonlinear oscillator driven by a nearly resonant force and by weak noise. Such an oscillator is a reasonably good model of a few physical systems, including optically bistable systems, and in particular a relativistic electron trapped in a Penning trap and driven by cyclotron radiation [12]. We emphasize that the onset of caustics in this system is not related to bistability that emerges in a comparatively strong field and was investigated in Ref. [9]. This is seen from the pattern of optimal paths shown in Fig. 1. The variables q_1, q_2 are the (dimensionless) coordinate and momentum of the oscillator in the rotating frame. The equations of motion in this frame are of the form (1) (cf. Ref. [9]), with

$$K_1 = q_2(q_1^2 + q_2^2 - 1) - \eta q_1,$$

$$K_2 = -q_1(q_1^2 + q_2^2 - 1) - \eta q_2 + \sqrt{\beta}.$$

Here, η is a dimensionless friction coefficient, and $\beta^{1/2}$ is the dimensionless force amplitude (the bistability arises for $\beta > \eta^2$).

It follows from the definition of the optimal path as the most probable way to reach a given point that, if a point q can be reached along two (or more) paths, only one of them is physically meaningful: this is the path that provides an absolute minimum to the action $S_a(q)$. We show below that such a path has never touched a caustic.

We first consider monostable systems, with the attractor a being the only steady state in the absence of noise. In this case the auxiliary Hamiltonian system has only one fixed point ($q = q_a, p = 0$). The trajectories ($q(t), p(t)$) (4) emanating from this point at $t \to -\infty$ form a smooth flow (cf. Ref. [13]) on a two-dimensional Lagrangian manifold (LM) [14]. Except for special cases (like detailed balance, $\nabla \times K = 0$) the projections of LM onto the original
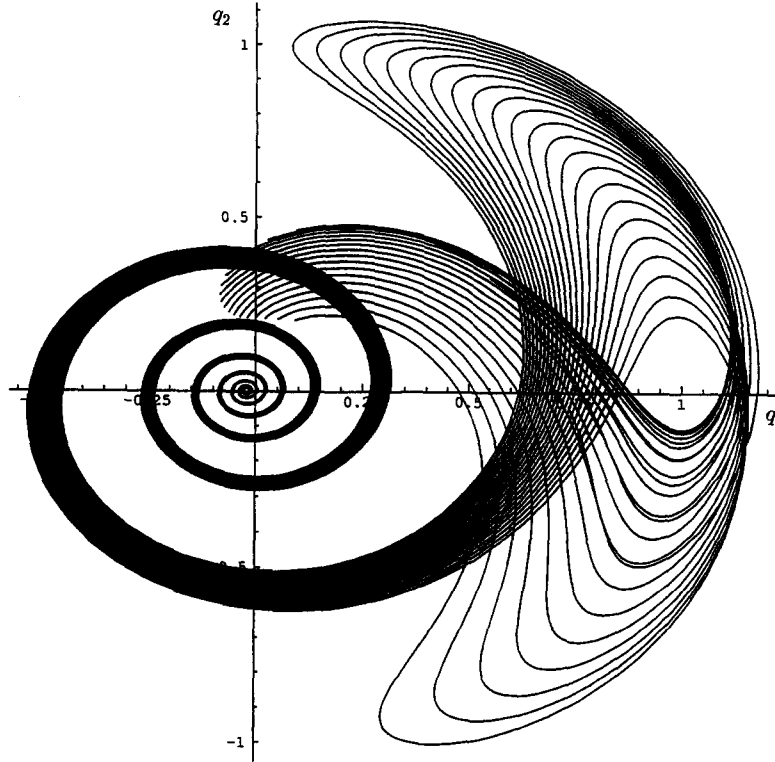
Fig. 1. Pattern of optimal paths of a periodically driven monostable nonlinear oscillator, $\eta = 0.1$ and $\beta = 0.0005$.

two-dimensional plane (q_1, q_2) will generally have singularities.

In two dimensions the only structurally stable types of singularities [15] are folds and cusps, as illustrated in Fig. 2. The projections of the folds of the LM are caustics. Each cusp gives rise to a pair of folds, and in the case under consideration folds can only begin or end at a cusp, or at infinity. This pattern is clearly seen in the plot of the optimal paths of a periodically driven oscillator in Fig. 1.

It is a feature of the dynamics (3), (4) that the Lagrangian is nonnegative definite. Thus, the action always increases along the extremal paths. This corresponds, quite naturally, to a decrease in probability density as the system moves along the path away from the attractor. An analysis which makes use of the normal form of the action near a caustic [14] and of the explicit form of the Hamiltonian $\mathcal{H}$ leads to an explicit local expression for the action. From this it can be seen [16] that the action to reach a point along a path

which *has not* touched a caustic *is always less* than that along a path which *has passed* through a caustic.

Near a cusp from which the caustics are going away (a "direction" of a caustic is that of the paths for which the caustic is an envelope) the probability distribution can be obtained by modifying the appropriate results of the WKB approximation in quantum mechanics [5]:

$$\rho_a(q) \propto \exp\left(-\frac{\boldsymbol{p}_c \cdot \boldsymbol{q}}{D}\right)$$

$$\times \int_{-\infty}^{\infty} dP_1 \exp\left(\frac{\tilde{S}(P_1, q_2) - P_1 q_1}{D}\right),$$

$$\tilde{S}(P_1, q_2) = -\tfrac{1}{4}a_{11}P_1^4 - \tfrac{1}{2}a_{12}P_1^2 q_2 - \tfrac{1}{2}a_{22}q_2^2. \qquad (5)$$

Here, q_1, q_2 are the coordinates measured from the cusp point $\boldsymbol{q}_c = 0$ along the directions transverse to, and parallel to the caustics at this point, i.e., the velocity of the path in the cusp is pointing along q_2,

S is a smooth function on LM

(a)   Lagrangian
cusp   2   manifold

fold

(b)   q-plane

2

caustic

S is multivalued with singularities on q-plane

(c)   action
                                surface
                          2
                                spinode edge
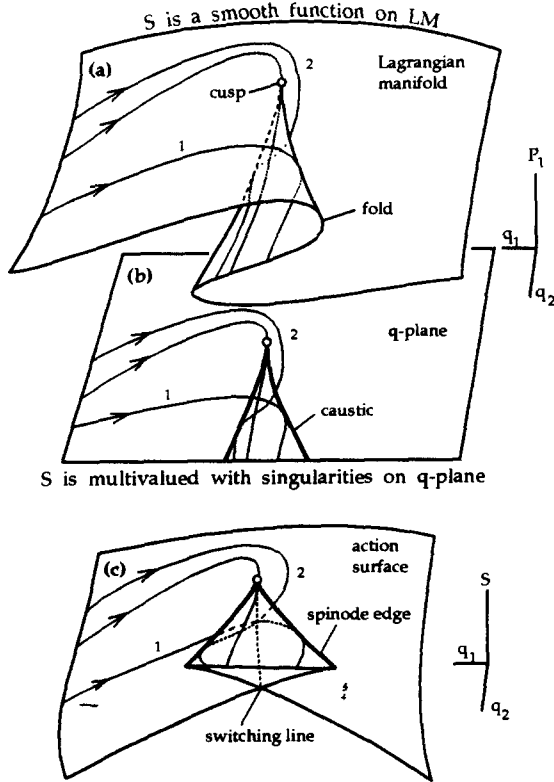
switching line

Fig. 2. Generation of singularities.

$v_c \equiv (\dot{q})_c = (0, v_c)$; $p_c = -K(q_c) + v_c$, $a_{12} = -v_c^{-1}$, $a_{22} = \partial[(2v_c)^{-1}K^2 - K_2]/\partial q_2$ (the derivatives of K are evaluated at the cusp point). The parameter a_{11} depends on the global features of the flow of the trajectories. It determines how sharply the caustics $q_1 = \pm 2a_{11}(q_2/3v_c)^{3/2}$ diverge with the distance from the cusp q_2. The prefactor in the probability distribution (2) blows up near the cusp point like $D^{-1/4}$.

For $|q_1|/D^{3/4}$, $|q_2|/D^{1/2}$ large and not close to the caustics the integral (5) can be evaluated by the steepest descent method, and the action $S_a(q)$ in (2) can be expressed in terms of $\tilde{S}(P_1, q_2)$ by implying $q_1 = \partial \tilde{S}/\partial P_1$. For $q_2 < 0$ the action $S_a(q)$ is single valued. On the other side of the cusp point, between the caustics, the action has three values, that is, the surface $S_a(q)$ has three sheets as shown in Fig. 2c. The top sheet, the one with the largest S_a, corresponds to the middle sheet of the LM in Fig. 2a. It is formed by the paths which have been reflected from one of the caustics, and contains the path which passes through

the cusp point. The two other sheets of the surface S_a and of the LM are formed by the paths which have not touched a caustic.

Only the solution with the smallest $S_a(q)$ should be kept in (2) in the range of q where the distance between the sheets of $S_a(q)$ greatly exceeds D. Therefore the top sheet of $S_a(q)$ is "invisible" away from the cusp, and the trajectories coming to the middle sheet of the LM in Fig. 2 drop out of the game. Two lower sheets of the action, $S_a^{(1)}$ and $S_a^{(2)}$, which correspond to the lower and upper sheets of the LM, intersect along a line with the projection $q_1^{(s)}(q_2)$ on the q-plane: $S_a^{(1)}(q_1^{(s)}, q_2)) = S_a^{(2)}(q_1^{(s)}, q_2)$. This line starts at the cusp point and lies between the coalescing caustics. There occurs switching at this line: the points a small distance from each other, but lying on different sides of it are reached along topologically different optimal paths $q(t)$ (those providing $S_a^{(1)}$ or $S_a^{(2)}$). They approach the switching line from opposite sides.

The switching line can be immediately observed via experiments [17] on the probability distribution of the paths $q(t)$ along which the system arrives to a given point. If this distribution is measured for various positions of the final point, its shape will change sharply once the final point crosses the switching line. We notice that caustics may *not* be observed via experiments of this sort, they are *hidden*: switching to another path occurs *prior* to a caustic being encountered.

The stationary distribution $\rho_a(q)$ is regular in the vicinity of a switching line: away from the cusp point it is given by

$$\rho_a(q) = \sum_{i=1,2} c^{(i)}(q) \exp[-S_a^{(i)}(q)/D], \qquad (6)$$

where the prefactors are evaluated for the paths lying on the different sheets of the LM. However, the derivative of $D \ln \rho_a$ transverse to the switching line is discontinuous in the limit $D \to 0$. This discontinuity was considered by Graham and Tèl [18], and by Jauslin [6] and Day [7]. The switching lines were found numerically in Ref. [6].

It is clear from the above picture that two switching lines emanating from different cusp points can end in a point where they intersect each other, and then another switching line starts at this point. Therefore there arise physically observable trees of switching lines, with the "free" ends at cusp points. Yet another con-

clusion concerns the possibility, expected on physical grounds, to reach *any point* (q_1, q_2) along an optimal path which has never touched a caustic. This possibility follows from the fact that caustics are the only lines that limit the flow of the optimal paths $q(t)$ in the considered case, and they emerge from the cusp points simultaneously with the switching lines. In particular the above results provide an insight into the switching to a new escape path observed in Ref. [8] when the old escape path is crossed by a cusp point as a parameter is varied.

The structure of the singularities becomes more complicated if a system has other steady states. A state of particular interest is an unstable stationary state: a saddle point q_s ($K(q_s) = 0$, $\det(\partial K_i/\partial q_j) < 0$, and we assume $\nabla \cdot K < 0$). Saddle points occur on the basin boundaries in multistable systems. In such systems, in addition to the characteristic relaxation time t_{rel} of the deterministic motion (that in the absence of noise), fluctuations about an initially occupied attractor a are characterized by the reciprocal probability W_a^{-1} of the noise-induced escape from the basin of attraction. In the time interval $t_{rel} \ll t \ll W_a^{-1}$ the probability distribution $\rho_a(q)$ is quasistationary far from the other attractors. We assume the basin boundary (the separatrix) to extend to infinity and to contain only one unstable stationary point q_s. It is the slowing down of the optimal path near q_s that gives rise to the effects we discuss.

The point $q = q_s$, $p = 0$ is a fixed point of the Hamiltonian equations (4), and close to it they can be linearized. We shall enumerate the eigenvectors $\{q^{(n)}, p^{(n)}\}$ ($n = 1, \ldots, 4$) so that the ones with $n = 1, 2$ are "fluctuational", $p^{(1,2)} \neq 0$, while the ones with $n = 3, 4$ are "deterministic", $p^{(3,4)} \equiv 0$ (the solution or (4) with $p = 0$ corresponds to the deterministic motion, $\dot{q} = K$). In the vicinity of the fixed point

$$q(t) = q_s + \sum_{n=1}^{4} C^{(n)} \exp(\lambda^{(n)} t) q^{(n)} \qquad (7)$$

and similarly $p(t) = \sum C^{(n)} \exp(\lambda^{(n)} t) p^{(n)}$; $\lambda^{(1,2)}$ are the eigenvalues of the matrix $-\partial K_i/\partial q_j$ evaluated in the saddle point, and $\lambda^{(4,3)}$ are their negatives. We choose

$$\lambda^{(1)} > \lambda^{(3)} > 0, \quad \lambda^{(2)} = -\lambda^{(3)},$$
$$\lambda^{(4)} = -\lambda^{(1)}. \qquad (8)$$

The optimal path of particular importance is the one along which the system escapes from the attractor. In a quite general case of a system driven by Gaussian noise the most probable escape path (MPEP) [10] ends up in the saddle point [4]. Since MPEP approaches the saddle point as $t \to \infty$, for this path $C^{(1)} = C^{(3)} = 0$ in (7). The interrelation between the coefficients $C^{(2)}$, $C^{(4)}$ is determined by the motion far away from the saddle point (in special cases, like detailed balance, $C^{(4)} = 0$). Because $|\lambda^{(4)}| > |\lambda^{(2)}|$, MPEP is tangent to $q^{(2)}$ in the saddle point (cf. Ref. [10]), and for q lying on the MPEP

$$q \times q^{(2)} = M(q \cdot q^{(2)})^{\lambda} q^{(4)} \times q^{(2)},$$
$$\lambda = \lambda^{(1)}/\lambda^{(3)} \qquad (9)$$

(we chose the direction of $q^{(2)}$ such that $C^{(2)} > 0$ for the MPEP).

For the extremal paths other than MPEP $C^{(1,3)} \neq 0$. The coefficients $C^{(1,3)}$ are interrelated via the expression $C^{(1)}C^{(4)}/C^{(2)}C^{(3)} = r$ where the constant r can be found from the condition that the energy of the Hamiltonian motion $E = 0$. The paths infinitesimally close to MPEP ($|C^{(1)}| \to 0$) and lying on the opposite sides of it approach asymptotically the eigenvectors $\pm q^{(1)}$ as $t \to \infty$ and then go away from the saddle point. The corresponding limiting paths form a "cut" of the LM. The singularities related to the cut which are of central interest here have not been considered in the analysis of the escape probability [10,19] where the absorbing boundary was placed along the vector $q^{(4)}$ (the basin boundary in the absence of fluctuations).

If the cut was not crossed by other optimal paths emanating from a given attractor a it would determine the range that can be reached from this attractor along an optimal path. However, crossing of the cut by the paths that have not encountered a caustic *may occur*, and in general, for $\lambda < \frac{3}{2}$ a *caustic emanates from the saddle point* tangent to the cut. The equation for the caustic $\partial(q_1, q_2)/\partial(t, \mu) = 0$ (μ is the parameter that "enumerates" the paths, the coordinate on a path $q \equiv q(t, \mu)$) can be solved for small $C^{(1,3)}$ (but $|C^{(4)}| \exp(\lambda^{(2)} t) \ll |C^{(1)}| \exp(\lambda^{(1)} t)$). The resulting interrelation between the coordinates of the caustic transverse and parallel to $q^{(1)}$ is of the form
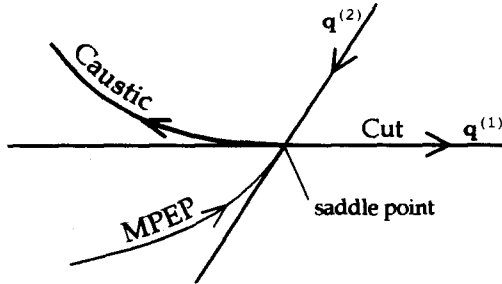
Fig. 3. Saddle point.

$$q \times q^{(1)} = \frac{2 - \lambda}{\lambda - 1} \left(\frac{\zeta}{M} q \cdot q^{(1)} \right)^{\alpha} q^{(1)} \times q^{(2)}, \quad (10)$$

where $\alpha = 1/(2 - \lambda)$, $1 < \lambda < \frac{3}{2}$, and

$$\zeta = \lambda(1 - \lambda) \frac{(p^{(1)} \cdot q^{(4)})(q^{(1)} \times q^{(3)})}{(p^{(2)} \cdot q^{(3)})(q^{(1)} \times q^{(2)})}$$

(the cross-product $q^{(i)} \times q^{(j)}$ has only one nonzero component, it is perpendicular to the q-plane, and we mean the ratio of the corresponding components by the ratio of the cross-products). Eq. (10) shows that the caustic is tangent to the cut in the saddle point and is described by a simple power law with the *exponent* $1 < \alpha < 2$ determined by *local* parameters of the motion near the saddle point. The inequality $\alpha < 2$, or $\lambda < \frac{3}{2}$ follows from the condition that the corrections to (10) due to nonlinearity be small and gives the criterion for the onset of the caustic [16]. The prefactor in (10) depends on the nonlocal characteristic M.

The general conclusion that optimal paths do not encounter caustics applies to the caustic emanating from the saddle point as well. The paths "beating" the ones approaching the caustic emanate from the saddle point themselves. When a system is approaching q_s its motion is slowed down, and it spends a time $\sim (1/\lambda^{(1)}) | \ln D |$ performing small fluctuations about q_s. Over this time a large fluctuation can occur which will drive the system away from q_s. It is then necessary to compare the probability to arrive at a given q directly from the attractor or via q_s, and it can be shown that the second scenario wins on the caustic. The switching line emanates from q_s and lies between the cut and the caustic. The system arrives on opposite sides of it (as well as on the opposite sides of the cut on the other side of the saddle point, cf. Fig. 3) di-

rectly from the attractor or having reached the saddle point first.

In conclusion, we have established the global structure of the pattern of optimal paths for dissipative Markov systems and revealed singular features related to the saddle points. We have shown why and how optimal paths avoid caustics. The singularities that can be immediately observed experimentally by tracing optimal paths or by measuring the probability distribution are switching lines. They start at the cusp points from which caustics emanate or at the saddle, and can form trees.

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