Transition-Rate Theory for Nongradient Drift Fields

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Classical transition-rate theory provides analytic techniques for computing the asymptotics of a weakly perturbed particle's mean residence time in the basin of attraction of a metastable state. If the dynamics of the particle are derivable from a potential, it typically escapes over a saddle point. In the nonpotential case exit may take place over an unstable point instead, leading to unexpected phenomena. These may include an anomalous pre-exponential factor, with a continuously varying exponent, in the residence time asymptotics. Moreover, the most probable escape trajectories may eventually deviate from the least-action escape path.

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Escape processes driven by weak external noise arise naturally in a multitude of physical, chemical, and engineering contexts. When the escaping particle moves in a space of two or more dimensions, there are analytic techniques [1, 2] for computing the weak-noise asymptotics of the mean time to exit the basin of attraction of a metastable point, and what is formally the most probable exit path (MPEP): the exiting classical trajectory of least action. These techniques apply to the most frequently studied case: when the dynamics of the particle, in the zero-noise limit, are specified by an irrotational (gradient) drift field, derivable from a potential. Here the MPEP typically extends along the unstable manifold of a hyperbolic equilibrium point (i.e., saddle) located on the "separatrix," the boundary of the basin.

The more general case, when the motion of the particle may be governed by a nongradient drift field, has received less attention [3–8]. Such drift fields can arise from coarse graining over variables whose underlying dynamics are not time-reversal invariant. A likely example may be activated processes in glasses, observed on scales on which there is no clear separation between the relaxation rates of coupled degrees of freedom [9]. Stochastically modeled communication networks provide another example [10].

In this Letter we begin a new study of the nongradient escape problem. We confine ourselves to a situation which cannot arise in the gradient case: when the exiting trajectory of least action terminates on an unstable equilibrium point on the boundary. We find a rich phenomenology, which differs in many ways from the case of exit over a saddle.

Techniques developed for the case of exit over a saddle are inapplicable here, and only partial results have been obtained [6, 7]. We have developed a general method for treating escape processes [11]. It clarifies the new phenomena that can arise, including the following: (i) A limiting exit location density concentrated not at an equilibrium point, but rather spread out over whole segments of the boundary, due to a splayout of exit trajectories. (ii) A limiting exit location density concentrated not at the point on the boundary where the least-action exit trajectory terminates, but at adjacent hyperbolic points. So the true MPEP need not coincide with the formal MPEP, the exiting classical path of least action. After reaching the boundary, it may move sideways along it until the hyperbolic points are reached. (iii) For the mean exit time, an anomalous temperature-dependent pre-exponential factor with a continuously varying exponent (considered as a function of the parameters of the drift field). These phenomena differ from anything known from standard transition-rate theory [2].

Our approach can be understood as a physical optics approximation, which exploits the formal similarities...
between the exit problem and classical Hamilton-Jacobi theory [3]. In the gradient case this similarity facilitates a WKB treatment, based on the approximation that the probability density is concentrated in a well-defined tube centered on the MPEP [1]. This picture can break down in the general case. We use matched asymptotic expansions, but in the context of a scaling Ansatz along the MPEP and the separatrix which does not assume a simple rule for falloff or growth of the probability in transverse
directions.

The model.—We specialize to the case of overdamped two-dimensional dynamics. A point particle
governed by the drift field \( \mathbf{u}(x, y) \) and subjected to thermal noise \( \mathbf{w}(t) \) has Langevin equation

\[
dx_i(t) = u_i(\mathbf{x}(t)) \, dt + \epsilon^{1/2} \, dW_i(t), \quad i = x, y
\]

with \( \epsilon = 2T \) the noise strength at temperature \( T \). The Fokker-Planck equation for the probability density \( \rho = \mathcal{L}^* \rho \), with \( \mathcal{L}^* \rho \) defined to equal \( (\epsilon^2/2)\Delta \rho - \partial_x (p u_x) - \partial_y (p u_y) \). If absorbing boundary conditions are imposed on the separatrix, the quasistationary density is defined [8] as the slowest decaying density mode, the eigenfunction \( \rho_1 \) of \( \mathcal{L}^* \) whose eigenvalue \( \lambda_1 \) has the greatest
real part. \( \lambda_1 \) is negative and converges to zero exponentially as \( \epsilon \to 0 \), so in the weak-noise limit the mean exit time \( \langle \tau_{\text{exit}} \rangle \), which may be approximated by \( (1/\lambda_1)^{-1} \), displays Arrhenius (i.e., exponential) growth. If \( \Omega \) denotes the basin and \( \partial \Omega \) the separatrix,

\[
\lambda_1 = \int_{\partial \Omega} (\epsilon/2) \partial_\nu \rho_1 \, dt \bigg/ \int_{\Omega} \rho_1 \, dx \, dy,
\]

(2)

since the right-hand side is the flux of probability through \( \partial \Omega \). If \( \lambda_1 \) is computed from this formula, its leading asymptotics, including the pre-exponential factor, will be unaffected [8] if \( \rho_1 \) is taken to satisfy \( \mathcal{L}^* \rho_1 = 0 \).

We consider the case of a drift field \( \mathbf{u}(x, y) \) symmetric about the \( x \) axis and with the structure shown in Fig. 1; more general cases can be handled by introducing curvilinear coordinates [11, 12]. The point \( (x_0, 0) \) is metastable, and the right-half plane is its basin of attraction. The separatrix is the \( y \) axis. The origin is an unstable point, and there are hyperbolic points at \( (0, \pm y_0) \); their unstable manifolds terminate on the metastable point. We expand \( \mathbf{u} \) near the \( z \) axis in \( y \):

\[
x_x = v_0(x) + v_2(x) y^2 + o(y^2),
\]

(3)

\[
x_y = u_1(x) y + o(y).
\]

(4)

Similarly, we expand \( \mathbf{u} \) near the \( y \) axis in \( x \). We write \( \lambda_1(S), \lambda_y(S), \lambda_2(U), \lambda_y(U), \lambda_2(H), \lambda_y(H) \) for the (real) eigenvalues of the drift field linearized at the metastable, unstable, and hyperbolic points; for example, \( \lambda_y(S) = u_1^2(x_0) \) and \( \lambda_y(H) = \partial_x v_0(y)/\partial_y v_0(y) \).

Away from the separatrix we may use the standard WKB approximation, \( \rho_1(x, y) \sim K(x, y) \exp[-W(x, y)/\epsilon] \) [8]. \( K(x, y) \) satisfies a transport equation, and \( W(x, y) \) an eikonal (Hamilton-Jacobi) equation: \( H(\mathbf{x}, \nabla W) = 0 \), with \( H \) the Wentzel-Freidlin Hamiltonian [3, 13],

\[
H(\mathbf{x}, \mathbf{p}) = \mathbf{p}^2/2 + V(\mathbf{x}) \cdot \mathbf{p}.
\]

(5)

So \( W(x, y) \), sometimes called the nonequilibrium potential [3], is the action of the zero-energy classical trajectory from \( (x_0, 0) \) to \( (x, y) \). If the zero-energy trajectory from \( (x_0, 0) \) to \( (0, 0) \) is the exit trajectory with least action, the MPEP will lie along the \( x \) axis and will terminate on the unstable point. This is the case we consider.

Asymptotic expansions.—To evaluate (2) we must approximate \( \rho_1 \) near the metastable point and separatrix. We take \( \rho_1(x, y) \sim \exp[-(\lambda_2(S)|x-x_0|^2 + |\lambda_y(S)y|^2)/\epsilon] \) near \( (x_0, 0) \). This Gaussian WKB approximation permits the evaluation of the denominator of (2). It is \( \pi \epsilon / \sqrt{\lambda_2(S) \lambda_y(S)} + o(\epsilon) \).

Near the MPEP and the separatrix, i.e., the \( x \) and \( y \) axes, we employ boundary layer expansions (cf. [8]). We use the scaling Ansatz

\[
\rho_1(x, y) \sim K(z) \int_{z_s}^{z} \gamma(z)^{1/2} \exp[-f_0(z)/\epsilon] \, dz
\]

(6)

with \( (x, z_s) = (x, y) \) and \( (y, z) \) for the \( x \) and \( y \) axes, respectively. This Ansatz assumes only that \( \rho_1 \) varies on an \( O(\epsilon^{1/2}) \) length scale in the transverse direction, and (away from equilibrium points) on an \( O(\epsilon) \) length scale in the longitudinal direction. Insertion of (6) into \( \mathcal{L}^* \rho_1 = 0 \) yields, after some work, the result that the boundary layer functions \( f_k^{(\epsilon)}(w) \) must be solutions of

\[
f'' + (\epsilon f)' + \delta f = 0,
\]

(7)

and are therefore related to one of the parabolic cylinder (p.c.) functions \( y_{i \pm} \), \( i = 1, 2 \), of Abramowitz and Stegun [14] by \( f_k^{(\epsilon)}(w) = y_{i \pm}(\mp i \delta - \epsilon, w) \exp(\mp iw^2/4) \). The index \( i \) is yet to be determined, as are \( \delta_x, \delta_y \), the \( \pm \) signs \( \pm_x, \pm_y \), and the functions \( K^{(x)}, f_0^{(x)}, \gamma^{(x)}, K^{(y)}, f_0^{(y)}, \gamma^{(y)} \).

On physical grounds we use the odd p.c. function \( y_2 \) when constructing the boundary layer function near the separatrix, and choose \( \pm_y = - \). With these choices \( \rho_1 \) will equal zero when \( x = 0 \) and will increase rapidly away from the separatrix. Similarly, we use the even p.c.
function $y_1$ when constructing the solution near the $x$ axis, and choose $\pm \delta_x = +$ (i.e., probability density falls off in the transverse direction) and $\delta_x = 0$ (implying a Gaussian profile). So near the $x$ axis

$$\rho_1(x, y) \sim K(x) \exp[-(f_0(x) + f_2(x)y^2)/\epsilon].$$  \(8\)

Here we have introduced $f_2 = \pm \gamma^2/2$, an alternative measure of transverse behavior. $f_2(x)$ must equal $\frac{1}{2}\partial^2 W/\partial y^2(x, 0)$ if our Ansatz (6) is to match up with the standard WKB approximation away from the $x$ axis; this follows from the asymptotics of the p.c. functions. [Similarly, $f_2^{(y)}(y)$ must equal $\frac{1}{2}\partial^2 W/\partial x^2(0, y)$.] $f_2(x)$ specifies the transverse length scale on which probability density decreases, so (8) resembles a WKB tube solution [1].

**Analysis.**— Substituting the Ansatz (6) into $\mathcal{L}^* \rho_1 = 0$ and equating powers of $\epsilon$, using (7) to simplify terms, yields equations for the functions $f_0, f_2, K$. (We drop the $z$ superscript unless necessary.) The first of these is the eikonal equation $H(z, f_0'(z)) = 0$, where $H(z, p_z) = p_z^2/2 + v_0(z)p_z$ is a Hamiltonian governing motion along the $z$ axis ($z = x$, $y$). This says that $f_0'(z)$ is the momentum of an on-axis classical trajectory with zero energy. There are two possibilities: $f_0'(z) = -2v_0(z)$ [arising from an "instanton" trajectory moving against the drift [15], with $z = -v_0(z)$], and $f_0 = 0$ [arising from an anti-instanton trajectory, with $z = +v_0(z)$]. The former is used along the $x$ axis, and the latter along the $y$ axis. We also get

$$f_2 = -2f_2^2 - 2v_1f_2 - v_0f_0', \quad K/K = -u_1 - (1 \pm \delta)f_2 - |v_0|\alpha_1.$$  \(9\)

$$K/K = -u_1 - (1 \pm \delta)f_2 - |v_0|\alpha_1.$$  \(10\)

The dot signifies derivative with respect to instanton or anti-instanton transit time, and the final term in (10) is present only in the anti-instanton case. Equation (10) is strictly correct only in the anti-instanton case or when $\delta = 0$, but those are the two cases we need.

To compute the normal derivative $\partial_x \rho_1(0, y)$ (which gives the exit location density), and the numerator of (2), we need to compute $\gamma^{(y)}$ (or $f_2^{(y)}$) and $K^{(y)}$. We solve first for $f_0^{(y)}, f_2^{(y)}, K^{(y)}$, and then determine $f_2^{(y)}$ and $K^{(y)}$ by requiring that our $x$- and $y$-axis approximations match together at the origin. The $x$-axis instanton has $\dot{z} = -v_0^{(x)}(x)$; it approaches $(x, 0)$ as $t \to -\infty$, and $(0, 0)$ as $t \to \infty$. For (8) to match with the Gaussian approximation near $(x, 0)$, $f_2^{(x)}$ must satisfy $f_2^{(x)}(x) = |\lambda_y(S)|$. Let $\mu$ denote $\lambda_y(U)/\lambda_x(U)$. If $v_0^{(x)}(x) = O(x^{2m-1}), z \not= 0$, which is often the case [11], it follows by integrating Eqs. (9) and (10) from $x = x_0$ toward $x = 0$ that $f_2^{(x)}(x) \sim Cx^{2m}$ and $K^{(x)}(x) \sim Cx^{2m}$ for certain $C, C'$. These asymptotics indicate that the WKB tube centered on the MPEP typically *splays out* as the unstable point is approached. This analysis assumes that the WKB tube is well defined along the entire MPEP, which will be the case unless $f_2^{(x)}(x^*) = 0$ for some $x^* > 0$. If a focusing singularity [16, 17] of this sort occurs along the MPEP, the tube bifurcates before it reaches the separatrix. Focusing singularities are easily checked for numerically; we disregard them in what follows.

Since $f_0^{(x)}(x) \sim -\lambda_x(U)x^2$ as $x \downarrow 0$, by restricting Eq. (8) to the $x$ axis we see that $\rho_1(x, 0)$ has asymptotics $C'x^\mu \exp[\lambda_y(U)x^2/\epsilon]$ as $x \downarrow 0$. This will match up with our $y$-axis approximation only if $\delta_y = -\mu$, $f_2^{(y)}(y) = -\lambda_x(U)$, and $K^{(y)}(0)$ is proportional to $e^{\mu/2} \exp[-f_0^{(y)}(0)/\epsilon]$. These follow from the fact that $y_2(\frac{1}{2} - \delta, w)$ is asymptotic to $(2/\pi)^{1/2} w^{-6} \exp(w^2/4)$ as $w \to +\infty$.

We can now integrate Eqs. (9) and (10) along the $y$ axis from $y = 0$ to $y = y_0$ to obtain the functions $f_2^{(y)}$ and $K^{(y)}$. The solution $f_2^{(y)}$ of (9) has an undetermined constant, but it can be shown [11] by considering the classical action $W(x, y)$ that the matching of the $x$-axis and $y$-axis Ansätze near the origin requires that $f_2^{(y)}(y) = -\lambda_x(U) + Cy^2 + o(y^2)$ if $\mu = 1$, and $f_2^{(y)}(y) = -\lambda_x(U) + o(y^2)$ if $\mu > 1$. So if $\mu = 2$, functions $f_2^{(y)}$ and $K^{(y)}$ are completely determined, and may be worked out numerically. (We defer the $\mu < 1$ case.)

**Our main taxonomy.**— It is useful to consider the behavior of the function $f_2^{(y)}$. Because $f_0^{(y)} = 0, f_2^{(y)}$ satisfies $\dot{f}_2 = -2f_2^2 - 2u_1^{(y)}f_2$. The time derivative here is with respect to the transit time of the $y$-axis instanton [the solution of $\dot{y} = +v_0^{(y)}(y)$]; its trajectory approaches $(0, 0)$ as $t \to -\infty$, and $(0, y_0)$ as $t \to \infty$. Since $f_2^{(y)}(0) = -\lambda_x(U)$, the initial condition is that $f_2^{(y)}(t = -\infty)$ equals $-\lambda_x(U)$. But since $u_1^{(y)} > 0$ for all $y$, $f_2^{(y)} < 0$ at all times. By the qualitative theory of differential equations, there are only three possibilities.

(1) $f_2^{(y)} \equiv$ constant. This can only occur if $u_1^{(y)}$, the repulsion of the separatrix at $(0, y)$, is independent of $y$, and $\mu > 1$. We defer this case until later.

(2) $f_2^{(y)} \to -\infty$ at finite time; i.e., $f_2^{(y)}(y^*) = -\infty$ for some $y^*$ between 0 and $y_0$. This will occur if $u_1^{(y)}$ decreases as $y$ increases, i.e., the repulsion of the separatrix lessens toward the hyperbolic points. Numerical studies suggest that when a divergence occurs, it is a sign that the zero-energy trajectory between $(x_0, 0)$ and $(0, y^*)$ is not unique. This is a focusing singularity [11, 17].

(3) $f_2^{(y)} \to 0$ as $t \to \infty$; equivalently, as $y \uparrow y_0$. This will occur if $u_1^{(y)}$ increases as $y$ increases, i.e., the repulsion of the separatrix strengthens toward the saddle.

The last case is the most straightforward. We know that $K^{(y)}(t = -\infty)$, i.e., $K^{(y)}(0)$, is proportional to $e^{\mu/2}$; it also contains the Arrhenius factor $\exp[-f_0^{(y)}(0)/\epsilon]$. By integrating (10) forward in time, we see the same is true for all $K^{(y)}(y)$ with $y$ between 0 and $y_0$. This has implications for the asymptotics of $t_{\text{exit}}$. Since differentiating our $y$-axis Ansatz for $\rho_1(x, y)$ with respect to $x$ pulls out a factor $\epsilon^{-1/2}$, the numerator of (2) contains a $\epsilon^{(1+\mu)/2}$ prefactor, as well as the Arrhenius factor. The
The denominator is proportional to $\epsilon$, so the $\lambda_1$ prefactor is proportional to $\epsilon^{(\mu-1)/2}$, and

$$
\langle t_{\text{exit}} \rangle \sim C'' \epsilon^{(\mu-1)/2} \exp \left( \frac{2}{\epsilon} \int_0^x v_0(x') \, dx' \right)
$$

(11)

with $C''$ computable. The form of the Arrhenius factor here follows from the fact that $f_0^{(y)^*} = -2v_0^{(x)}$.

The prefactor in (11) is anomalous. Its exponent varies continuously, and depends only on $\mu$. This dependence on the ratio of eigenvalues at the unstable point occurs despite the fact that the limiting exit location density is nonzero everywhere between the two hyperbolic points. $[It$ is proportional to $\partial_x \rho_1(0, y)$, i.e., to $K(y)|f(y)|^{1/2}$, and can be computed numerically.]

**Special cases.**—The above taxonomy dealt with certain subcases of the $\mu \geq 1$ case. There are two cases, which we term quasi-one-dimensional, where the computation of the asymptotics of $\langle t_{\text{exit}} \rangle$ and the exit location density requires either a more general Ansatz or results on one-dimensional exit times. The instanton trajectory $\hat{x} = -v_0^{(x)}(x)$, formally, has infinite transit time between $(x_0, 0)$ and $(0, 0)$. But Day [7] has shown that when finally exiting, the particle follows the instanton trajectory only until it gets within an $O(\epsilon^{1/2})$ distance of the separatrix. The final fluctuation of the particle, beginning an $O(1)$ distance away and terminating on the separatrix, therefore requires $2\lambda_x(U)^{-1} \ln(1/\epsilon) + O(1)$ time. In general this must be compared with the logarithmic time scale introduced by Suzuki [18], which in the present context is the time needed for the particle’s probability density, moving out along the WKB tube toward the separatrix, to separate from the transversely unstable MPEP into two distinct peaks. Suzuki’s time is $[2\lambda_y(U)^{-1} \ln(1/\epsilon) + O(1)$, and a further time $[2\lambda_y(H)^{-1}]^{-1} \ln(1/\epsilon) + O(1)$ is required for the two peaks to become localized around the hyperbolic points.

So if $\lambda_y(U) < \lambda_x(U)$, i.e., $\mu < 1$, the splaying out of the tube is only apparent: the splayout terminates when $x = O(\epsilon^{1/2})$, and as $\epsilon \to 0$ the exit location on the separatrix converges to the unstable point. By the small-$x$ asymptotics of $f_2^{(y)}(x)$, which by (8) governs the tube width, $y = O(\epsilon^{1-\mu/2})$ at exit time. So the $\mu < 1$ case is quasi-one-dimensional. A computation of the flux of probability through the separatrix, as in (2), reveals that $\langle t_{\text{exit}} \rangle$ has asymptotics

$$
\frac{\pi}{C' \epsilon^{-1/2} \sqrt{\lambda_x(S)\lambda_y(S)\lambda_x(U)}} \exp \left( \frac{2}{\epsilon} \int_0^x v_0(x') \, dx' \right).
$$

The prefactor displays a novel dependence on the vector field $\vec{u}$ along the entire MPEP. The asymptotics of the exit location density and the quasistationary distribution, on the length scales $x = O(\epsilon^{1/2})$ and $y = O(\epsilon^{1-\mu/2})$, can also be worked out [7,11].

The other quasi-one-dimensional case is $\mu \geq 1$, with $u_1^{(y)}$ independent of $y$. Here the WKB tube splays out, but to leading order the repulsion of the separatrix is independent of position, so $x(t)$ and $y(t)$ decouple near the separatrix. The above formula for $\langle t_{\text{exit}} \rangle$ still holds, and it is possible to draw detailed conclusions about the exit position from the relative sizes of the Day (longitudinal) and Suzuki (transverse) time scales. Unlike $\mu < 1$, $y$ will not be $O(1)$ at exit time. There are four subcases.

(1) $\lambda_x(U)^{-1} = \lambda_y(U)^{-1}$, i.e., $\mu = 1$. The time scales are comparable: as $\epsilon \to 0$, the exit location density will have a nonzero limit on the interval from $(0, -y_h)$ to $(0, y_h)$. We have already treated this case: the limiting density is proportional to $K(y)|f_2^{(y)}(y)|^{1/2}$.

(2) $\lambda_y(U)^{-1} < \lambda_x(U)^{-1} < \lambda_y(U)^{-1} + |\lambda_y(H)|^{-1}$. The Suzuki time scale is shorter, but the particle does not have time to reach the diffusion-dominated region of width $O(\epsilon^{1/2})$ around the hyperbolic points before it exits. By comparing the Day time scale with the transit time of the $y$-axis anti-instanton, we see that $y - y_h$ (respectively, $y + y_h$) will be $O(\epsilon^\mu)$ at exit time, with $\zeta$ equal to $\xi \lambda_y(U)^{-1} - \lambda_x(U)^{-1}$. The limiting exit location density, on the $O(\epsilon^\mu)$ length scale, will be "skewed": located entirely on the small-$|y|$ side of the saddle.

(3) $\lambda_x(U)^{-1} = \lambda_y(U)^{-1} + |\lambda_y(H)|^{-1}$. This is a crossover case: the particle reaches the diffusive region around one of the hyperbolic points before it exits, but in the remaining $O(1)$ time its $y$ coordinate does not have time to thermalize. We expect a non-Gaussian exit location distribution, with an $O(\epsilon^{1/2})$ standard deviation.

(4) $\lambda_x(U)^{-1} > \lambda_y(U)^{-1} + |\lambda_y(H)|^{-1}$. The particle enters the diffusive region before it exits, and $y$ has time to thermalize. So in the $\epsilon \to 0$ limit $y - y_h$ (respectively, $y + y_h$) will be normally distributed at exit time, with standard deviation equal to $\epsilon^{1/2}/\sqrt{2|\lambda_y(H)|}$. The crossover from the skewing regime to Gaussian behavior was predicted by Day [7], but our crossover criterion is new.

**Example.**—$u(x, y) = (x - x^2, (1 - 2x^2)y - y^2)$ is a simple quasi-one-dimensional drift field with the topology of Fig. 1: $x_0 = 1, y_h = 1, \mu = 1$. The solution of the eikonal equation $H(\vec{z}, \nabla W) = 0$, with $H$ the Hamiltonian of Eq. (5), is by examination $W(x, y) = -x^2 + x^2 + 2x^2y^2 + 1/2$. The zero-energy trajectory from $(1, 0)$ to $(0, 0)$ is the only one emanating from $(1, 0)$ which exits the right half-plane. So it is the formal MPEP.

That $f_2^{(x)}(x) = x^2$ and $f_2^{(y)}(y) = -1 + y^2$ is easily checked. $K(y)$ follows by integrating the transport Eq. (10) along the boundary, using $\pm \zeta = -\delta_y = -\mu = -1$. We get $K(y) \propto (1 - y^2)^{-1/2}$.

Since $K(y)f_2^{(y)}(y)^{1/2}$ is a constant function of $y$, for this drift field $\vec{u}$ the limiting exit location density is uniform between $(0, -1)$ and $(0, 1)$. The MPEP extends from $(1, 0)$ to $(0, 0)$, and then branches sideways. As $\epsilon \to 0$, exit may take place at any point between the two hyperbolic points with equal probability.

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