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Critical diffusions

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by Edward Nelson

The proper setting for this discussion is a Riemannian manifold, but I want to avoid complications due to curvature, boundary conditions, and regularity conditions, so I will work on the flat torus $\mathbb{T}^n = \mathbb{R}^n/\mathbb{Z}^n$ and will assume everything to be C^∞.

1. Stochastic Hamilton-Jacobi theory

Let $\phi\colon \mathbb{T}^n \times \mathbb{R} \longrightarrow \mathbb{R}$ and $A\colon \mathbb{T}^n \times \mathbb{R} \longrightarrow \mathbb{R}^n$ be C^∞. We call ϕ the scalar potential and A the vector potential. Define the corresponding Lagrangean $L\colon \mathbb{T}^n \times \mathbb{R}^n \times \mathbb{R} \longrightarrow \mathbb{R}$ by

$$L(x,p,t) = \frac{1}{2}\, p\cdot p - \phi(x,t) + A(x,t)\cdot p$$

where the dot denotes the Euclidean inner product on $\mathbb{R}^n$. The space $\mathbb{T}^n$ may be thought of as the configuration space of a system of particles, and their masses are absorbed into the Euclidean inner product for simplicity of notation.

By a smooth Markovian diffusion on $\mathbb{T}^n$, with diffusion constant $\hbar$ and forward drift b, where $b\colon \mathbb{T}^n \times \mathbb{R} \longrightarrow \mathbb{R}^n$ is C^∞, is meant a $\mathbb{T}^n$-valued Markov process ξ such that for all C^∞ functions $f\colon \mathbb{T}^n \times \mathbb{R} \longrightarrow \mathbb{R}$,

$$Df(\xi(t),t) = \left(\frac{\hbar}{2}\, \Delta + b(\xi(t),t)\cdot\nabla + \frac{\partial}{\partial t}\right) f(\xi(t),t) ,$$

where D is the stochastic forward derivative

$$Df(\xi(t),t) = \lim_{dt \to 0+} E_t\, \frac{f(\xi(t+dt),t+dt) - f(\xi(t),t)}{dt}$$

(with E_t the conditional expectation given $\xi(t)$).

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For $t < t_1$ in $\mathbb{R}$ and ν a natural number, let $s_\alpha = t+\alpha(t_1-t)/\nu$ for $\alpha = 0,\ldots,\nu$, let $ds_\alpha = (t_1-t)/\nu$, let $d\xi(s_\alpha) = \xi(s_\alpha+ds_\alpha)-\xi(s_\alpha)$, and let $s_\alpha^o = (s_{\alpha-1}+s_\alpha)/2$. A smooth Markovian diffusion ξ with diffusion constant $\hbar$ and forward drift b is <u>critical for the Lagrangean</u> L in case it is indexed by $\mathbb{R}$ and for all $t < t_1$ in $\mathbb{R}$, whenever $\delta b\colon T^n \times [t,t_1] \longrightarrow \mathbb{R}^n$ is C^∞ and ξ' is the smooth diffusion indexed by $[t,t_1]$ with diffusion constant $\hbar$, forward drift $b' = b+\delta b$, and the same probability distribution at time t as ξ, then

$$\lim_{\nu\to\infty} \{E\sum_{\alpha=1}^{\nu}[\frac{1}{2}\frac{d\xi(s_\alpha)}{ds_\alpha}\cdot\frac{d\xi(s_\alpha)}{ds_\alpha} -\phi(\xi(s_\alpha^o),s_\alpha^o)ds_\alpha+A(\xi(s_\alpha^o),s_\alpha^o)\cdot d\xi(s_\alpha)]$$

$$- E\sum_{\alpha=1}^{\nu}[\frac{1}{2}\frac{d\xi'(s_\alpha)}{ds_\alpha}\cdot\frac{d\xi'(s_\alpha)}{ds_\alpha} -\phi(\xi'(s_\alpha^o),s_\alpha^o)ds_\alpha+A(\xi'(s_\alpha^o),s_\alpha^o)\cdot d\xi'(s_\alpha)]\} = o(\delta b) .$$

Notice the order of operations in this definition: first we take the Riemann sums for the action integral, then we take the expectation, then we take the variation, and only at the end do we take the limit as the mesh of the partition tends to 0.

If $\hbar = 0$, this reduces to the usual definition in Hamilton-Jacobi theory for the flow generated by b to be critical for the Lagrangean L. In this case it is known that ξ is critical for L if and only if the Hamilton-Jacobi condition

$$b+A = \nabla S$$

holds, where S is Hamilton's principal function, and consequences of this are the Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t} +(\nabla S-A)\cdot(\nabla S-A)-\phi = 0$$

and the Newton equation

$$a = F$$

(see the previous comment about masses), where a is the acceleration $a = \ddot{\xi}$ and the force is

$$F = E+H\cdot p$$

where $E = -\nabla\phi - \frac{\partial A}{\partial t}$, H is the exterior derivative of A , and

$$(H\cdot p)_i = \sum_j \left(\frac{\partial A_j}{\partial x^i} - \frac{\partial A_i}{\partial x^j}\right)p^j .$$

Theorem 1. *Let* $\hbar > 0$. *Then a smooth Markovian diffusion* ξ *with diffusion constant* $\hbar$ *and forward drift* b *is critical for* L *if and only if there is a solution* ψ *of the Schrödinger equation*

1) $i\hbar \frac{\partial\psi}{\partial t} = [\frac{1}{2} (\frac{\hbar}{i} \nabla - A)\cdot(\frac{\hbar}{i} \nabla - A)+\phi]\psi$

such that

2) $b = (\mathrm{Re}+\mathrm{Im})\hbar\nabla\log \psi - A$.

Proof. First let us examine the kinetic contribution to the action. Let $dt > 0$ and for any function f of time let $df(t) = f(t+dt)-f(t)$. Then

3) $d\xi(t) = \int_t^{t+dt} b(\xi(s),s)ds+dw(t)$

where w is the Wiener process on $\mathbf{T}^n$ with diffusion constant $\hbar$ (infinitesimal generator $\frac{\hbar}{2}\Delta$ and probability density 1). We may estimate this as $b(\xi(t),t)dt+dw(t)+o(dt)$, but this is not accurate enough if we wish to estimate

$$\frac{1}{2}\frac{d\xi}{dt}\cdot\frac{d\xi}{dt}$$

to $o(1)$, since $dw(t)$ is of order $dt^{\frac{1}{2}}$. (Notice that $d\xi/dt$ is a quotient, not a derivative.) But apply (3) to itself; i.e., to $\xi(s)$ in the integrand. Then

$$d\xi(t) = \int_t^{t+dt} b(\xi(t)+\int_t^s b(\xi(r),r)dr+w(s)-w(t),s)ds+dw(t) ,$$

so that

$$d\xi(t) = b(\xi(t),t)dt + \sum_k \frac{\partial}{\partial x^k} b(\xi(t),t)W^k + dw(t) +o(dt^{3/2})$$

where $W^k = \int_t^{t+dt} [w^k(s)-w^k(t)]ds$. These terms are of order dt , $dt^{3/2}$, and $dt^{\frac{1}{2}}$ respectively. Therefore

$$\frac{1}{2}\frac{d\xi}{dt}\cdot\frac{d\xi}{dt} = \frac{1}{2}b\cdot b+ \frac{b\cdot dw}{dt} + \frac{1}{dt^2} \sum_k \frac{\partial b}{\partial x^k} W^k\cdot dw+ \frac{1}{2}\frac{dw}{dt}\ \frac{dw}{dt} +o(1) .$$

The term $b\cdot dw/dt$ is of order $dt^{-\frac{1}{2}}$, but $E_t b\cdot dw = 0$. Now if $t \leq s \leq r$, then

$$E_t[w^k(s)-w^k(t)][w^i(r)-w^i(t)] = (s-t)\hbar\delta^{ki} ,$$

so that

$$E_t \frac{1}{dt^2} \sum_k \frac{\partial b}{\partial x^k} W^k\cdot dw = \frac{\hbar}{2}\nabla\cdot b$$

and $E_t dw\cdot dw = \hbar n dt$. Therefore

4) $$E_t \frac{1}{2}\frac{d\xi}{dt}\cdot\frac{d\xi}{dt} = \frac{1}{2}b\cdot b+ \frac{\hbar}{2}\nabla\cdot b+ \frac{\hbar n}{2dt} +o(1) .$$

A smooth diffusion with strictly positive diffusion constant has a C^∞ strictly positive probability density ρ , since the probability distribution is a weak and positive (and hence C^∞ and strictly positive) solution of the forward Fokker-Planck equation

$$\frac{\partial \rho}{\partial t} = \frac{\hbar}{2}\Delta\rho - \nabla\cdot(b\rho) \ .$$

Then we also have

$$D_* f(\xi(t),t) = \left(-\frac{\hbar}{2}\Delta + b_*(\xi(t),t)\cdot\nabla + \frac{\partial}{\partial t}\right) f(\xi(t),t)$$

for any C^∞ function $f\colon \mathbb{T}^n \times \mathbb{R} \longrightarrow \mathbb{R}$, where D_* is the stochastic backward derivative

$$D_* f(\xi(t),t) = \lim_{dt \to 0+} E_t \frac{f(\xi(t),t) - f(\xi(t-dt),t-dt)}{dt} ,$$

and the backward drift b_* is determined by the osmotic equation

$$\frac{b-b_*}{2} = \frac{\hbar}{2}\nabla \log \rho ,$$

whose left hand is called the <u>osmotic velocity</u>, denoted by u. The <u>current velocity</u> v is defined by

$$v = \frac{b+b_*}{2} ;$$

it satisfies the current equation (or equation of continuity)

$$\frac{\partial \rho}{\partial t} = -\nabla\cdot(v\rho) \ .$$

These assertions are proved in [2,pp. 104-106].

Now let us examine the vector potential contribution to the action. We have

$$EA(\xi(s^o_\alpha),s^o_\alpha)\cdot d\xi(s_\alpha) = EA(\xi(s^o_\alpha),s^o_\alpha)\cdot v(\xi(s^o_\alpha),s^o_\alpha)ds_\alpha + o(ds_\alpha) ,$$

but

$$5)\quad EA\cdot v = \int A\cdot v\rho = \int A\cdot b\rho - \int A\cdot u\rho = \int A\cdot b\rho - \int A\cdot \frac{\hbar}{2}\nabla\rho = \int A\cdot b\rho + \frac{\hbar}{2}\int \nabla\cdot A\rho$$

$$= E\left(A\cdot b + \frac{\hbar}{2}\nabla\cdot A\right) \ .$$

Let us define the stochastic forward Lagrangean $L_+ : \mathbb{T}^n \times \mathbb{R} \longrightarrow \mathbb{R}$ by

$$L_+ = \frac{1}{2}\, b\cdot b + \frac{\hbar}{2}\, \nabla\cdot b - \phi + A\cdot b + \frac{\hbar}{2}\, \nabla\cdot A \ .$$

By (4) and (5)

$$EL_+(\xi(t),t) = E\Big[\frac{1}{2}\,\frac{d\xi}{dt}\cdot\frac{d\xi}{dt} - \phi(\xi(t),t) + A(\xi(t),t)\cdot \frac{\xi(t+dt)-\ (t-dt)}{2dt}\Big] - \frac{\hbar n}{2dt} + o(1) \ .$$

We define

$$I = E\int_t^{t_1} L_+(\xi(s),s)ds \ .$$

Then ξ is critical for L if and only if

$$I' - I = o(\delta b) \ ,$$

where quantities with ξ' replacing ξ are denoted by $'$. Notice that the term $\hbar n/2dt$ in (4), which tends to ∞ as $dt \longrightarrow 0$, disappears when we take the variation.

Let $E_{x,t}$ be the conditional expectation, given $\xi(t)$, for the process conditioned by $\xi(t) = x$, and define

$$S(x,t) = -E_{x,t}\int_t^{t_1} L_+(\xi(s),s)ds \ .$$

This is the stochastic analogue of Hamilton's principal function, and we have $DS = L_+$.

For the rest of the proof, we follow [1]. In fact, the contribution of this section is a comment on the work of Guerra and Morato, to the effect that we do not need to posit any stochastic Lagrangean; we may start with the usual Lagrangean. Here is the rest of the proof in outline: we have

$$D(S'-S) = D'S' - DS + (D-D')S' = L_+' - L_+ - \delta b\cdot\nabla S' = L_+' - L_+ - \delta b\cdot\nabla S + o(\delta b) \ .$$

Now $L'_+ - L_+ = (b+A)\cdot\delta b + \frac{\hbar}{2}\nabla\cdot\delta b + o(\delta b)$. Since S and S' vanish at t_1 , and ρ and ρ' are the same at t ,

$$-\int_t^{t_1} D(S'-S)ds = ES'(\xi(t),t) - ES(\xi(t),t) = E'S'(\xi'(t),t) - ES(\xi(t),t)$$

$$= -I'+I \ ;$$

but $I'-I = E\int_t^{t_1}(b+A-\nabla S+\frac{\hbar}{2}\nabla)\cdot\delta b ds + o(\delta b)$. Now

$$E\,\frac{\hbar}{2}\nabla\cdot\delta b(\xi(s),s) = \int\frac{\hbar}{2}(\nabla\cdot\delta b)\rho = -\int\delta b\cdot u\rho \ ,$$

and since $b-u = v$,

$$I'-I = E\int_t^{t_1}(v+A-\nabla S)\cdot\delta b ds + o(\delta b) \ .$$

We may take $\delta b = v+A-\nabla S$. Therefore ξ is critical for L if and only if the stochastic Hamilton-Jacobi condition

$$v+A = \nabla S$$

holds. Let

$$R = \frac{\hbar}{2}\log\rho \ ,$$

so that $\nabla R = u$ and $b = v+u = \nabla S-A+\nabla R$. If we write out $DS = L_+$ we obtain

$$\left(\frac{\partial}{\partial t} + b\cdot\nabla + \frac{\hbar}{2}\Delta\right)S = \frac{1}{2}b\cdot b + \frac{\hbar}{2}\nabla\cdot b - \phi + A\cdot b + \frac{\hbar}{2}\nabla\cdot A \ ,$$

and expressing everything in terms of R and S we find the stochastic Hamilton-Jacobi equation

$$\frac{\partial S}{\partial t} + \frac{1}{2}(\nabla S-A)\cdot(\nabla S-A) - \phi + \frac{1}{2}\nabla R\cdot\nabla R - \frac{\hbar}{2}\Delta R = 0 \ ,$$

which together with the current equation expressed in terms of R and S ,

$$\frac{\partial R}{\partial t} + \nabla R\cdot(\nabla S - A) + \frac{\hbar}{2}\Delta S - \frac{\hbar}{2}\nabla\cdot A = 0 \;,$$

gives a coupled system on nonlinear equations. But if we let

$$\psi = e^{\frac{1}{\hbar}(R+iS)} \;,$$

this system is equivalent to the Schrödinger equation (1). ■

A simple computation shows that the stochastic Newton equation

$$\frac{1}{2}(D_* b + D b_*) = E + H\cdot v$$

holds. The peculiar form $\frac{1}{2}(D_* b + D b_*)$ of the stochastic acceleration is no longer an assumption as in [2]; it is a consequence of the variational principle.

A change in the choice of the final time t_1 in the definition of S produces a guage transformation that leaves the process ξ and the stochastic Newton equation unchanged.

2. Zeros of the wave function

If ξ is a smooth Markovian diffusion that is critical for L, the corresponding solution of the Schrödinger equation is nowhere 0, by (2). In this section it will be shown that a diffusion process (not smooth in the sense of our definition) is still well-defined by (2) when ψ has zeros.

Let ψ be a C^∞ solution of (1) and let

$$Z_\varepsilon = \{(x,t) \in \mathbb{T}^n \times \mathbb{R}^+ : |\psi(x,t)| \le \varepsilon\} \,.$$

For $\varepsilon > 0$, the vector field b defined by (2) is C^∞ on Z_ε^c.

Let $\varepsilon > 0$, and for $0 \le s < t$ let $p_\varepsilon(x,s;y,t)$ be the solution of the forward Fokker-Planck equation on Z_ε^c with Dirichlet boundary conditions and initial value δ_x at time s. Then p_ε satisfies the Chapman-Kolmogorov equation

$$\int p_\varepsilon(x,s;y,t)p_\varepsilon(y,t;z,r)dy = p_\varepsilon(x,s;z,r) \ , \ s < t < r \ ,$$

but its integral (in y) is less than 1 . To remedy this, let $\dot{\mathbb{T}}^n = \mathbb{T}^n \cup \{\infty\}$ and define

$$p_\varepsilon(x,s;\{\infty\},t) = 1-\int p_\varepsilon(x,s;y,t)dy \ ;$$

then p_ε is a transition probability. Let χ_ε^c be the indicator function of Z_ε^c , and choose an initial measure $\rho_\varepsilon^o = \rho(o,y)\chi_\varepsilon^c(o,y)dy$ with $\rho_\varepsilon^o(\{\infty\}) = 1-\int\rho(o,y)\chi_\varepsilon^c(o,y)dy$, where $\rho = |\psi|^2$. (We may assume that $\int|\psi|^2 = 1$.) Let Pr_ε be the corresponding regular probability measure on path space

$$\Omega = \prod_{t\,\in\mathbb{R}^+} \dot{\mathbb{T}}^n$$

and let $\xi_\varepsilon(t)$ be the evaluation map $\omega \longmapsto \omega(t)$; then ξ_ε is a $\dot{\mathbb{T}}^n$-valued Markov process. The configuration diffuses with drift b until it hits Z_ε , when it is killed (sent to ∞) .

Let ρ_ε be the probability density of ξ_ε . Then $\rho_\varepsilon \leq \rho$ on $\mathbb{T}^n \times \mathbb{R}^+$, since both are positive solutions of the forward Fokker-Planck equation on Z_ε^c with the same initial value and $\rho_\varepsilon = 0$ on ∂Z_ε^c .

The p_ε are increasing in y on $\mathbb{T}^n$ as ε decreases. Let $p(x,s;y,t)$ be their limit, with $p(x,s;\{\infty\},t)$ the defect in its integral (we will show that this is 0) , and let Pr be the corresponding regular probability measure on Ω with initial measure $\rho(o,y)dy$. Let

$$D = \{\omega \in \Omega\colon \omega(t) = \infty \text{ for some } t \text{ in } \mathbb{R}^+\} \ .$$

Then $Pr_\varepsilon(D)$ decreases to $Pr(D)$.

<u>Theorem 2</u>. $Pr(D) = 0$.

<u>Proof</u>. Let $0 < T < \infty$ and let $D_T = \{\omega \in \Omega\colon \omega(t) = \infty$ for some t

in $[0,T]\}$. Then we need only show that $\Pr_\varepsilon(D_T)$ decreases to 0 . Throughout this proof, time parameters are restricted to lie in $[0,T]$.

Let us set $\hbar = 1$, so that $|\psi| = e^R$. Let

$$X(t) = R(\xi_\varepsilon(t),t)-R(\xi_\varepsilon(0),0) \ ,$$

with the convention that $R(\infty) = 0$. By the continuity of paths, D_T is equal $\Pr_\varepsilon$ - a.e. to $\{\inf R(\xi_\varepsilon(t),t) = \log \varepsilon\}$, so we need only establish bounds on $\Pr_\varepsilon\{\sup |X(t)| > \lambda\}$ that are independent of ε and tend to 0 as $\lambda \longrightarrow \infty$.

Now

$$X(t) = \int_0^t dR(\xi_\varepsilon(s),s) = \int_0^t [\frac{\partial R}{\partial s}\, ds + b\cdot\nabla R ds + \frac{1}{2}\, \Delta R ds + \nabla R\cdot dw(s)]$$

where by convention each term in the integrand is 0 after the killing time. Call the four integrals $X^\alpha(t)$ for $\alpha = 1,2,3,4$. Then X^4 is a martingale, so (since $\nabla R = u$)

$$\Pr_\varepsilon\{\sup |X^4(t)| > \lambda\} \le \frac{1}{\lambda^2}\int_0^T \int u\cdot u\rho_\varepsilon dt \le \frac{1}{\lambda^2}\int_0^T \int u\cdot u\rho dt \ .$$

Let $H_0(t) = -\frac{1}{2}\,(\frac{1}{i}\,\nabla - A)\cdot(\frac{1}{i}\,\nabla - A)$. Then a simple computation shows that

$$(\psi, H_0(t)\psi) = \frac{1}{2}\int (u\cdot u + v\cdot v)\rho \ .$$

Thus X^4 is OK, by which I mean that $\Pr_\varepsilon\{\sup |X^4(t)| > \lambda\}$ is bounded independently of ε by a bound that tends to 0 as $\lambda \longrightarrow \infty$. Clearly, X^2 is OK. Now

$$\Pr_\varepsilon\{\sup |X^3(t)| > \lambda\} \le \frac{1}{\lambda}\int_0^T \int |\frac{1}{2}\,\Delta R|\rho dt \ ,$$

but

$$\int |\frac{1}{2}\,\Delta R|\rho = \frac{1}{4}\int |\nabla\cdot\rho^{-1}\nabla\rho|\rho = \frac{1}{4}\int |-\rho^{-2}\nabla\rho\cdot\nabla\rho + \rho^{-1}\Delta\rho|\rho \le \int u\cdot u\rho + \int |\Delta\rho| \ ,$$

so X^3 is OK. Finally,

$$\Pr_\varepsilon\{\sup |X^1(t)| > \lambda\} \leq \frac{1}{\lambda}\int_0^T \int \left|\frac{\partial R}{\partial t}\right| \rho_\varepsilon dt = \frac{1}{\lambda}\int_0^T \int \chi_\varepsilon^c \, \frac{1}{2} \left|\frac{\partial \rho}{\partial t}\right| \rho^{-1} \rho_\varepsilon dt$$

$$\leq \frac{1}{\lambda}\int_0^T \int \frac{1}{2} \left|\frac{\partial \rho}{\partial t}\right| dt$$

so X^1 is OK. The diffusion never reaches the zeros of the wave function.

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References

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[2] Edward Nelson, Dynamical Theories of Brownian Motion, Princeton University Press, Princeton, 1967.