

Use of Hamiltonian mechanics in systems driven by colored noise

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The evaluation of the path-integral representation for stochastic processes in the weak-noise limit shows that these systems are governed by a set of equations which are those of a classical dynamics. We show that, even when the noise is colored, these may be put into a Hamiltonian form which leads to improved numerical treatments and to better insights. We concentrate on solving Hamilton's equations over an infinite time interval, in order to determine the leading order contribution to the mean escape time for a bistable potential. The paths may be oscillatory and inherently unstable, in which case one must use a multiple shooting numerical technique over a truncated time period in order to calculate the infinite time optimal paths to a given accuracy. We look at two systems in some detail: the underdamped Langevin equation driven by external exponentially correlated noise, and the overdamped Langevin equation driven by external quasimonochromatic noise. We deduce that the bifurcation of the optimal path in the latter case is due to singularities in the configuration space of the corresponding dynamical system.

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I. INTRODUCTION

The subject of noise induced activation has received a great deal of attention in the past decade or so with the development of new techniques which allow systems where the noise is not white (i.e., colored) to be studied in a systematic and controlled way [1-4]. While these techniques were being refined it was natural that only the simplest of systems were studied: those which consisted of a single particle moving in a one-dimensional potential with a relatively simple form of noise. More recently the investigation of models acted upon by white noise and having more than one degree of freedom has revealed novel effects such as caustics and focusing singularities [5-9]. In these systems it was also found that the leading order term in the expression for the mean escape time, that is, the action, was reduced unexpectedly [7].

The appearance of such features can be understood in the following way. In the limit of weak noise the dynamics of the system is governed by a set of equations which are the extrema of the action in the path-integral formulation of the stochastic process. These equations have the same form as those of Newtonian mechanics, if the original stochastic dynamics was underdamped and the noise was white. Hence the dynamics of these stochastic processes is controlled by trajectories in a $2n$ -dimensional phase space, where n is the number of degrees of freedom of the system. By analogy with what is found in the WKB approximation in quantum mechanics [10], we would expect caustics or focusing singularities to appear due to instanton trajectories intersecting each other. Within the Hamiltonian formalism these appear when trajectories in phase space are projected down onto configuration space [11]. In fact, since the Lagrangian that appears in the path-integral formulation of stochastic processes [see, for example, (5) later] is non-negative, there are differences to what is found in quantum mechanics [9]. Nevertheless, multidimensional systems, without detailed balance and

acted upon by white noise, will typically have singularities in configuration space. In this paper we will show that similar effects can also be expected to occur in systems with one degree of freedom, but with a more complicated type of noise. To study such effects it is useful, both from a practical (i.e., numerical) and a conceptual point of view, to introduce a generalized Hamiltonian formalism. In this way a phase space can be constructed which is multidimensional and hence, since these systems do not satisfy detailed balance, one may be expected to see the phenomena mentioned above.

Our starting point is the observation that a system consisting of a single degree of freedom, but acted upon by a rather general form of external noise [12], can be written as a Markov process which consists of a number of equations, only one of which involves a noise term (which is white). These equations can be combined into a single equation, at the expense of introducing higher time derivatives. Essentially we have traded a simple system acted upon by a complicated noise term, for a complicated system acted upon by a simple white noise. We shall give explicit examples later in this paper. A process of the kind we have been describing can be defined by the generic stochastic differential equation

$$f(x, \dot{x}, \ddot{x}, \dots, x^{(n)}; t) = \eta(t), \quad (1)$$

where $\eta(t)$ is Gaussian white noise of strength D .

Let us now make the above comments on the emergence of a classical dynamics in the weak noise limit more concrete by outlining how a path-integral representation for the conditional probability distribution of a process defined by (1) can be written down [13]. One begins by using (1) to transform the probability density functional for white noise given by

$$P[\eta] = C \exp\left(-\frac{1}{4D} \int_{t_0}^t \eta^2(t) dt\right), \quad (2)$$

to the probability density functional for that of the coordinate x :

$$P[x] = \mathcal{N} J[x] \exp\left(-\frac{S[x]}{D}\right), \quad (3)$$

where $S[x]$ is the action mentioned above and $J[x]$ is the Jacobian of the transformation. The action is so called since it may be written as

$$S[x] = \int_{t_0}^t dt L(x, \dot{x}, \ddot{x}, \dots, x^{(n)}; t), \quad (4)$$

where $L(x, \dots)$ given by

$$L(x, \dot{x}, \ddot{x}, \dots, x^{(n)}; t) = \frac{1}{4} [f(x, \dot{x}, \ddot{x}, \dots, x^{(n)}; t)]^2. \quad (5)$$

This has the form of a Lagrangian for a mechanical system, if the noise is white and the motion is overdamped, so that no time derivatives higher than the first appear in (1). For colored noise processes of the type we are investigating here, there are higher time derivatives in the Lagrangian and the analogy is now with a generalized form of mechanics. The precise form of the Jacobian factor will not be required in this paper since we will be performing our calculations to leading order only and the Jacobian only enters at next order. Probability distributions, correlation functions, and other quantities of interest can be found by integration of the appropriate functions over paths $x(t)$ with weight (3). In the limit of $D \rightarrow 0$ these path integrals can be evaluated by the method of steepest descents, the paths which dominate the integrals being the ones for which $\delta S[x]/\delta x = 0$. This leads to the Euler-Lagrange equation for the optimum path which will be a $2n$ th-order nonlinear differential equation given by

$$\sum_{j=0}^n (-1)^j \frac{d^j}{dt^j} \left(\frac{\partial L}{\partial x^{(j)}} \right) = 0. \quad (6)$$

In general, this equation will have no analytical solution and one has to rely on numerical techniques [3, 14–16]. A numerical solution will involve the decomposition of such an equation into $2n$ coupled first-order nonlinear differential equations. It would be convenient to derive the an expression for the optimal path in such a format automatically. This is instantly provided by using Hamilton's formalism as an alternative to the Lagrangian method. We have already mentioned that the structure of Hamiltonian mechanics gives one a better insight into why the optimal paths take on the particular form they do. Now here is another, more practical, advantage.

The outline of the paper is as follows. In Sec. II we construct the generalized Hamiltonian formalism appropriate to problems of this type and give the case of the underdamped Langevin equation driven by white noise as an example. In Sec. III we use the formalism to find the mean first passage time for this underdamped problem, but now with exponentially correlated noise, a task which could not be achieved using the Lagrangian formalism [14]. The case of quasimonochromatic noise is discussed in Sec. IV and we conclude in Sec. V.

II. HAMILTONIAN FORMALISM

For a dynamical system which is defined by a Lagrangian of the form $L(x, \dot{x}, \ddot{x}, \dots, x^{(n)}; t)$, a Hamiltonian structure can still be constructed (see, for instance, [17]). To do so one introduces a generalized coordinate vector \vec{q} spanning an n -dimensional space with components $\{q_1, \dots, q_n\}$ such that

$$q_i = x^{(i-1)} \quad (7)$$

and one writes

$$L(x, \dot{x}, \ddot{x}, \dots, x^{(n)}; t) = \sum_{i=1}^n p_i \dot{q}_i - H(\vec{q}, \vec{p}; t), \quad (8)$$

where the p_i 's have yet to be defined. Now if one demands that $\dot{p}_i = -\partial H/\partial q_i$, it follows from (8) that

$$\frac{\partial L}{\partial x^{(j)}} = p_j + \dot{p}_{j+1}, \quad j = 0, \dots, n, \quad (9)$$

where p_0 and p_{n+1} are defined to be zero. From (6) and (9) one sees that the components $\{p_1, \dots, p_n\}$ of the generalized momentum vector \vec{p} should be taken to be

$$p_i = \sum_{j=i}^n (-1)^{j-i} \frac{d^{j-i}}{dt^{j-i}} \left(\frac{\partial L}{\partial x^{(j)}} \right). \quad (10)$$

Hence, by construction, the optimum path given by the $2n$ th-order differential equation (6) can also be found by solving the $2n$ first-order differential equations

$$\dot{q}_i = \frac{\partial H}{\partial p_i} \quad (11)$$

and

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}. \quad (12)$$

If the Lagrangian does not involve time explicitly, then the Hamiltonian H also has no explicit time dependence, and since $dH/dt = \partial H/\partial t$, the Hamiltonian is conserved. This reduces by one the number of integrals that have to be performed.

As an example we shall consider the underdamped Langevin equation driven by white noise

$$m\ddot{x} + \alpha\dot{x} + V'(x) = \eta(t), \quad (13)$$

where $\eta(t)$ is Gaussian white noise of strength D . Here $V(x)$ is assumed to be a double-well potential and α is a friction constant which will be set equal to unity by an appropriate choice of units of time. The Lagrangian for this process is given by

$$L(x, \dot{x}, \ddot{x}) = \frac{1}{4} [m\ddot{x} + \dot{x} + V'(x)]^2 \quad (14)$$

and the Hamiltonian is found to be

$$H(\vec{q}, \vec{p}) = p_1 q_2 + \frac{p_2^2}{m^2} - \frac{p_2}{m} [q_2 + V'(q_1)]. \quad (15)$$

The optimum path is then the solution of Hamilton's equations

$$\dot{q}_1 = q_2,$$

$$\dot{q}_2 = \frac{2p_2}{m^2} - \frac{q_2}{m} - \frac{V'(q_1)}{m},$$

$$\dot{p}_1 = \frac{p_2 V''(q_1)}{m},$$

$$\dot{p}_2 = \frac{p_2}{m} - p_1 \quad (16)$$

and the action is given by

$$S = \int_{t_0}^t \frac{p_2^2}{m^2} dt. \quad (17)$$

In this case we can find the required solutions explicitly enough to allow us to write down the action in closed form. We are searching for solutions that begin at extrema of the potential with all time derivatives of the coordinate equal to zero. This immediately tells us that $H = 0$ for these solutions, which is a common feature in models of this type. For this simple case there are only two of these solutions: a "downhill" solution given by $m\ddot{x} + \dot{x} + V'(x) = 0$ and an "uphill" solution given by $m\ddot{x} - \dot{x} + V'(x) = 0$ (see, for instance, [14]). These solutions can easily be found as $H = 0$ solutions of (16): the downhill solution has $p_1 = p_2 = 0$ and zero action and the uphill solution has $p_1 = V'(q_1)$, $p_2 = mq_2$, and action given by

$$S = \left[\frac{1}{2}mq_2^2 + V(q_1) \right]_{t_0}^t. \quad (18)$$

The interpretation of (18) depends on exactly what quantity is being calculated. For example, if one wished to find the stationary probability distribution, then one would take $t_0 \rightarrow -\infty$ so that $S = m\dot{x}^2/2 + V(x)$ in terms of the original variable x , which just gives the Maxwell-Boltzmann distribution. On the other hand, if one wished to find the mean escape rate from a potential well, one is interested in paths that take an infinite time to interpolate between stable and unstable points of the potential and are at rest at both ends. This gives $S = \Delta V$, where ΔV is the barrier height. For the rest of this paper we will restrict ourselves to the calculation of this quantity and so will assume an infinite time interval in what follows. Since for colored noise processes, which are the real interest of this paper, we cannot, in general, calculate the action explicitly, we will choose the specific double-well potential

$$V(x) = -\frac{x^2}{2} + \frac{x^4}{4} \quad (19)$$

to illustrate our techniques. If we choose to investigate activation from the left-hand well to the right-hand well, then the section from 0 to +1 will be a downhill path with zero action. Thus we need only concern ourselves with the section of the path from -1 to 0. Having illustrated the technique on a simple white noise problem we now go on to investigate the same system, but acted upon by exponentially correlated noise.

III. EXPONENTIALLY CORRELATED NOISE

In this section we consider the process modeled by the Langevin equation

$$m\ddot{x} + \dot{x} + V'(x) = \xi(t), \quad (20)$$

where $\xi(t)$ is Gaussian colored noise whose correlation function is given by

$$\langle \xi(t)\xi(t') \rangle = \frac{D}{\tau} \exp\left(-\frac{|t-t'|}{\tau}\right). \quad (21)$$

This represents the simplest generalization of the noise in the system first investigated by Kramers [18], which it reduces to in the $\tau \rightarrow 0$ limit. One can see that it is the simplest generalization by replacing (21) by the condition that ξ obeys the first-order differential equation

$$\tau\dot{\xi} + \xi = \eta(t), \quad (22)$$

where η is a Gaussian white noise of strength D . Equations (20) and (22) form an equivalent Markov process with two degrees of freedom. These equations may be combined into the single third-order stochastic differential equation

$$m\ddot{x} + \dot{x} + V'(x) + \tau[m\ddot{x} + \dot{x} + \dot{x}V''(x)] = \eta(t). \quad (23)$$

This is of the form (1) with $n = 3$ and so we expect to be able to describe the weak noise limit of this system using either Lagrangian or Hamiltonian dynamics.

The Lagrangian approach to this problem has been investigated by Newman *et al.* [14]. However, these authors were only able to explore the dynamics of the system for relatively small masses; they were unable to analyze the underdamped regime. We shall show in this section that the Hamiltonian approach allows us to do this.

Using (5) and (23) we can write down a Lagrangian for this system:

$$L(x, \dot{x}, \ddot{x}, \ddot{\ddot{x}}) = \frac{1}{4} \{ [m\ddot{x} + \dot{x} + V'(x)] + \tau[m\ddot{x} + \ddot{x} + \dot{x}V''(x)] \}^2. \quad (24)$$

The equivalent Hamiltonian is found in the way described in Sec. II to be:

$$H(\vec{q}, \vec{p}) = p_1 q_2 + p_2 q_3 + \frac{p_3^2}{m^2 \tau^2} - \frac{p_3}{m \tau} [m q_3 + q_2 + V'(q_1)] - \frac{p_3}{m} [q_3 + q_2 V''(q_1)] \quad (25)$$

with Hamilton's equations given by (11) and (12). The action reduces to

$$S = \int_{-\infty}^{\infty} dt \frac{p_3^2}{m^2 \tau^2}. \quad (26)$$

We now wish to find the value of the infinite time action for the bistable potential (19). The downhill solution is, as usual, trivial: $p_n = 0$, $n = 1, 2, 3$, which gives zero action. The uphill solution cannot be found analytically for general m and τ and only perturbative methods and numerical solutions are available. The $m = 0$, general τ

problem is extensively discussed in [3], along with perturbative expansions in the small τ and large τ regimes. Therefore we will restrict ourselves to $m > 0$. In Ref. [14] a numerical calculation of the action for certain values of m and τ has been given, as well as perturbation expansions for small m and small τ . In the rest of the section we will expand on this treatment, extending it and investigating the previously unexplored underdamped regime.

For general m , but small τ , the action for the uphill path has the form

$$S(m, \tau) = S_0 + \tau^2 S_1(m) + O(\tau^4), \quad (27)$$

where $S_0 = 1/4$ is the white noise action for this potential. The first correction $S_1(m)$ has the simple form [14]

$$S_1(m) = \int_{-\infty}^{\infty} \ddot{x}_0^2 dt, \quad (28)$$

where x_0 is the optimal path for white noise ($\tau = 0$) and is given by the nonlinear differential equation

$$m\ddot{x}_0 - \dot{x}_0 + V'(x_0) = 0 \quad (29)$$

with the boundary conditions $x_0(-\infty) = -1$ and $x_0(\infty) = 0$.

In the paper by Newman *et al.* [14] this quantity was calculated for small m only. However, Eq. (29) is stable if integrated backward in time, i.e., starting at $x_0 = 0$ going to $x_0 = -1$ (stability is discussed further when the full solution is considered). Hence one can use a simple initial value integrating scheme, such as a fourth-order Runge-Kutta, starting with an infinitely small velocity $\dot{x}_0 = \delta$. While in a formal sense the path over the infinite time interval is only found in the limit $\delta \rightarrow 0$, in practice we find that if δ is small, the value of the action does not depend on it. The results for $S_1(m)/S_0$ are plotted in Fig. 1 as a function of $\log_{10}(m)$. The dotted line shows a seventh-order perturbative calculation of $S_1(m)$:

$$S_1(m) = S_0 \left(\frac{1}{2} + \frac{m}{5} - \frac{m^2}{5} - \frac{2m^3}{5} + \frac{3m^4}{10} + \frac{9m^5}{5} - \frac{3m^6}{5} - \frac{778m^7}{55} \right) + O(m^8). \quad (30)$$

Figure 1 shows the excellent agreement between the series (30) and the numerical solution for m less than about 0.3, and the catastrophic failure of the series above that value. This breakdown of perturbation theory may be due to the change in the nature of the solutions that occurs at $m = 1/8$ (see below) and a calculation of more terms in the series (30) might show that the value of m at which the breakdown occurs approaches the value 0.125. This figure also shows that the value of $S_1(m)$ has a maximum when plotted against $\log_{10}(m)$. Such maxima are also seen when plotting actions against $\log_{10}(m)$ ([14] and Fig. 2 below). The existence of these maxima are a consequence of the nonlinear nature of the problem.

Now let us go on to a numerical study of the solution of Hamilton's equations for general m and τ . As a first step we linearize the equations about the end points $q_1 = a$, where a is 0 or -1 . To do this we approximate the potential by a parabola $V(q_1) = V(a) + \frac{1}{2}V''(a)(q_1 - a)^2$, which leads to linear Hamilton's equations with solutions

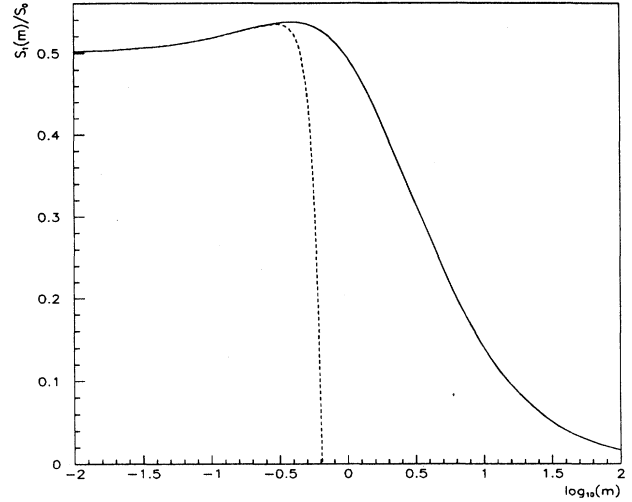


FIG. 1. $S_1(m)$ plotted against $\log_{10}(m)$.

of the form $q_1 = a + \sum_n A_n e^{\lambda_n t}$, where A_n are arbitrary constants specified by the boundary conditions. The λ_n have six possible values:

$$\lambda_n = \pm \frac{1}{\tau}, \pm \left(\frac{1}{2m} \pm \frac{\sqrt{1 - 4mV''(a)}}{2m} \right). \quad (31)$$

When $a = 0$, $V''(a) = -1$ and we require that $q_1 \rightarrow 0$ as $t \rightarrow \infty$ for an uphill path, so we select only those λ_n which are negative. Conversely, when $a = -1$, $V''(a) = 2$ and we require that $q_1 \rightarrow -1$ as $t \rightarrow -\infty$, thus we must only take values of λ_n which are positive, i.e.,

$$\lambda_{1,2,3} = \frac{1}{\tau}, \left(\frac{1}{2m} + \frac{\sqrt{1 - 8m}}{2m} \right), \left(\frac{1}{2m} - \frac{\sqrt{1 - 8m}}{2m} \right). \quad (32)$$

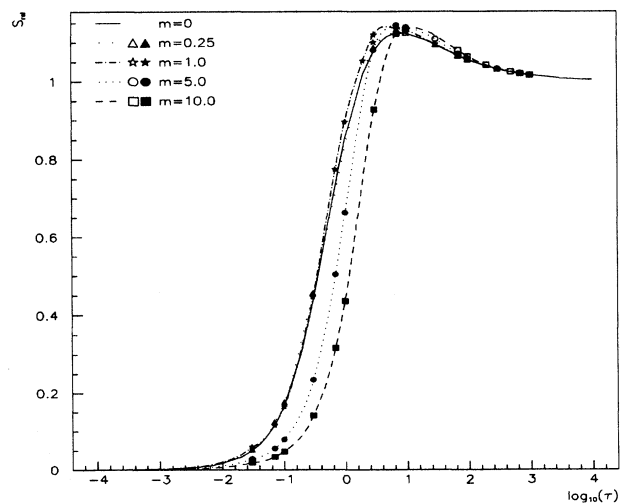


FIG. 2. $S_r(m, \tau)$ against $\log_{10}(\tau)$ for different values of m .

If $m < 1/8$, no problem arises. However, if $m > 1/8$, two of the quantities in (32) are complex, which is a signal that the solutions may be oscillatory. Actually, if $\tau > 2m$, the real one dominates, implying that the solutions are not oscillatory near the stable fixed point in this case. In summary, we can say that, as in the underdamped Langevin equation with white noise, the system oscillates about the bottom of the potential wells before making a transition, unless $m < 1/8$ or $m > 1/8$ and $\tau > 2m$. In this case the substitution $y(x) = \dot{x}(t)$, which was the basis of the approach in [14], fails and another technique has to be used.

The advantage of solving for $y(x)$ is that since $-1 \leq x \leq 0$, the differential equation has to be solved in a finite range. Unfortunately, in the region of parameter space where the oscillatory solution exists we have to solve Hamilton's equations over the range $-\infty < t < \infty$. In practice, of course, we have to truncate this span to a large, but finite, value T and use the boundary conditions

$$\begin{aligned} q_1\left(-\frac{T}{2}\right) &= -1, & q_1\left(\frac{T}{2}\right) &= 0, \\ q_2\left(\pm\frac{T}{2}\right) &= 0, \\ q_3\left(\pm\frac{T}{2}\right) &= 0 \end{aligned} \quad (33)$$

and calculate the action

$$S = \int_{-\frac{T}{2}}^{\frac{T}{2}} \frac{p_3^2}{m^2\tau^2} dt. \quad (34)$$

The extrapolation $T \rightarrow \infty$ is, in fact, not a problem; the actual transition happens over a time scale of order a few m and for the majority of the time the particle is almost at rest at the two end points. Furthermore, this decay of the position, velocity, etc., at the end points is exponential, which means that the truncation can be carried out extremely accurately. However, the simple initial value techniques of solution which are used in shooting routines can no longer be used as this problem is inherently unstable. This is because, as one can see from (31), there are growing solutions at both the end points. In analytic treatments these solutions can be ignored by setting the arbitrary constants (A_n) to zero. Numerically, roundup errors introduced either through machine precision or through the solution algorithm make these constants small, but nonzero. Since these solutions grow exponentially, whereas the required solution decays exponentially, they soon take over and any hope of solving the problem numerically by this method is destroyed.

Normally, it is possible to solve inherently unstable problems by using a relaxation technique or collocation such as COLSYS [19]. However, as noticed in Ref. [14], this technique is poorly convergent when the solution is oscillatory. Instead, one can attempt to proceed using either invariant embedding or multiple shooting techniques. It is the latter that we have used, calculating the action for $\tau < 2m$ using MUSN [20]. These techniques

damp out the exponentially growing solution by splitting the total time span into several smaller time segments and then matching the solution continuously [21]. In this regime it turns out that the time of integration T needs only to be of the order of a few m in order to obtain reliable results. On the other hand, if we try to find the solution as a function $x(t)$ in the regime $\tau > 2m$, the time of integration needs to be of the order of a few τ , which, since we are interested in large values of τ , becomes a problem. Fortunately, as we have seen, the solution can be found as a function $y(x)$ in this case.

The results of the numerical solution are shown in Fig. 2 for several values of the mass. It is convenient not to plot the action $S(m, \tau)$ itself, but the reduced quantity

$$S_r(m, \tau) = \frac{S(m, \tau) - S_0}{S_\infty(\tau)}, \quad (35)$$

since this is finite in the limits $\tau \rightarrow 0$ and $\tau \rightarrow \infty$, having the values 0 and 1, respectively. Here S_0 is the action when $\tau = 0$ and $S_\infty(\tau)$ is the action in the large τ limit and is given by [3]

$$S_\infty = \frac{2\tau}{27}. \quad (36)$$

S_0 and S_∞ are m independent. For $\tau > 2m$, the hollow points have been calculated using (y, x) variables and the solid points using (x, t) variables. The lines are curves of best fit through these points to aid the eye.

This figure shows that numerically the mass has little effect on the action and the overdamped Langevin equation provides an excellent approximation to the action for the underdamped system. There seems no reason to expect this *a priori*, except for the fact that since in the limit of small and large τ the action is m independent, there is very little freedom at intermediate values of τ to have significant deviations from the $m = 0$ result.

IV. QUASIMONOCROMATIC NOISE

In Secs. II and III two explicit types of noise have been considered: white noise whose power spectrum is flat and exponentially correlated noise which has a spectrum centered about zero. A type of noise that has a definite color, in the sense that it has a power spectrum peaked at a nonzero frequency, is quasimonochromatic noise (QMN) [22–26]. Systems acted upon by QMN are the subject of this section.

The noise $\xi(t)$ is defined by

$$\ddot{\xi} + 2\Gamma\dot{\xi} + \omega_0^2\xi = \eta, \quad (37)$$

where η is a Gaussian white noise of strength D . Hence, for the overdamped system $\dot{x} + V'(x) = \xi(t)$, the Lagrangian is given by

$$\begin{aligned} L(x, \dot{x}, \ddot{x}, \ddot{\xi}) &= \frac{1}{4} \left[[\dot{x} + V'(x)] + \frac{2\Gamma}{\omega_0^2} [\ddot{x} + \dot{x}V''(x)] \right. \\ &\quad \left. + \frac{1}{\omega_0^2} [\ddot{x} + \ddot{x}V''(x) + \dot{x}^2V'''(x)] \right]^2 \end{aligned} \quad (38)$$

and the Hamiltonian is found to be

$$H(\vec{q}, \vec{p}) = p_1 q_2 + p_2 q_3 + \omega_0^4 p_3^2 - p_3 \{ \omega_0^2 (q_2 + V') + 2\Gamma (q_3 + q_2 V'') + q_3 V''' + q_2^2 V'''' \}. \quad (39)$$

The dynamics will be governed, in the limit of weak noise, by solutions of Hamilton's equations given by (11) and (12). For concreteness we will again consider the potential to be of the form (19) and hence we will require the truncated infinite time boundary conditions (33) for the uphill path. The action for the uphill path will be given by

$$S = \int_{-\frac{T}{2}}^{\frac{T}{2}} \omega_0^4 p_3^2 dt. \quad (40)$$

The downhill path again leads to zero action and will not be considered further.

An analysis of the linearized Hamilton equations near the end points along the lines described in Sec. III again shows there to be oscillations depending on the value of Γ [in fact oscillations occur for $\Gamma < \min(2, \omega_0)$] and so once again we are unable to use the (y, x) parametrization of the solution. Figure 3 shows the generalized coordinates found by solving Hamilton's equations for $\Gamma = 0.45$ and $\omega_0 = 10$. This particular value of ω_0 was chosen to allow comparison with earlier work [26], where an approximate solution to the classical dynamics was used to calculate the action. The value of Γ is chosen for clarity: for smaller values it is harder to illustrate graphically a complete transition showing the smaller scale oscillatory features characteristic of QMN, whereas for larger values these oscillations are absent. As is already known, the paths have three distinctive features: (i) an underlying oscillatory factor of angular frequency ω_0 , (ii) an underlying growth and decay either side of the transition time t_0 given approximately by $\exp(-\Gamma|t - t_0|)$, and (iii) that they pass over the top of the potential barrier many times before coming to rest.

These features only occur if Γ is less than a critical value Γ_c (which has a value just less than $\frac{1}{2}$); otherwise the solution is that of the system acted upon by white

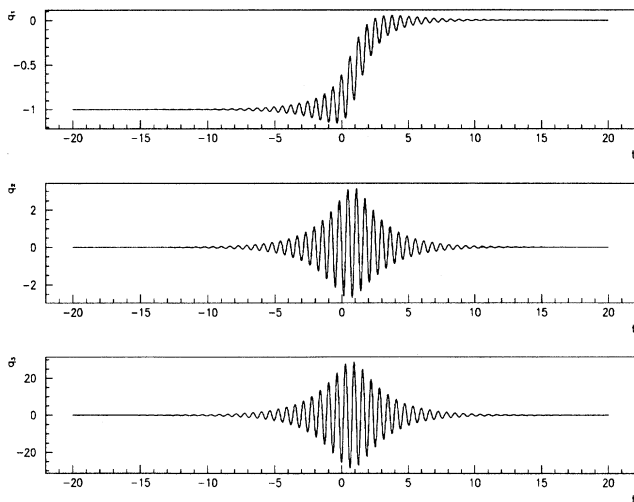


FIG. 3. q_1 , q_2 , and q_3 against t for $\Gamma = 0.45$ and $\omega_0 = 10$.

noise to an accuracy of 1% (i.e., of order $1/\omega_0^2$). They explain why the approximate treatment given in [26] was successful: there it was assumed that the paths had exactly the features (i) and (ii) above. The last point mentioned above shows that one has to distinguish clearly between a mean first passage and a well transition.

Figures 4 and 5 show the second and third figures of [26] redrawn with the action calculated from the Hamiltonian technique shown as a dotted line. The asterisk on the action S indicates that it is the most probable escape path — for $\Gamma < \Gamma_c$ the escape path can be either white-noise-like or oscillatory, but it is the latter that occurs in practice since it has the least action and so is most probable. These two figures show the remarkably good agreement between solving the full equations and the approximation used in [26]: the value of Γ_c is approximately the same and a maximum value of S^*/Γ occurs at $\Gamma \sim 0.1$. From Fig. 4 one can also see that for $\Gamma < \Gamma_c$, $S^* \approx \frac{2}{3}\Gamma$ and for $\Gamma > \Gamma_c$, $S^* \approx \frac{1}{4}$. The intersection of these lines gives $\Gamma_c = \frac{3}{8}$, which is a reasonable estimate.

Difficulties arise for small Γ as the time required for transition goes as Γ^{-1} and hence a longer time span T is required. If we attempt to rescale time by Γ , the frequency of oscillations now goes as ω_0/Γ , which means we need a finer grid of shooting points to calculate the action to sufficient accuracy. So far we have only been able to extend our method down to $\Gamma = 0.05$.

If one writes down an equation for the optimum path [given by Eq. (12) of [26]] perturbatively in powers of $1/\omega_0^2$, one finds that the uphill solution is

$$\dot{x} = V'(x) + O\left(\frac{1}{\omega_0^2}\right), \quad (41)$$

which has the corresponding action

$$S = \frac{1}{4} - \frac{1}{4\omega_0^2} + O\left(\frac{1}{\omega_0^4}\right). \quad (42)$$

This approximate solution is independent of the value of

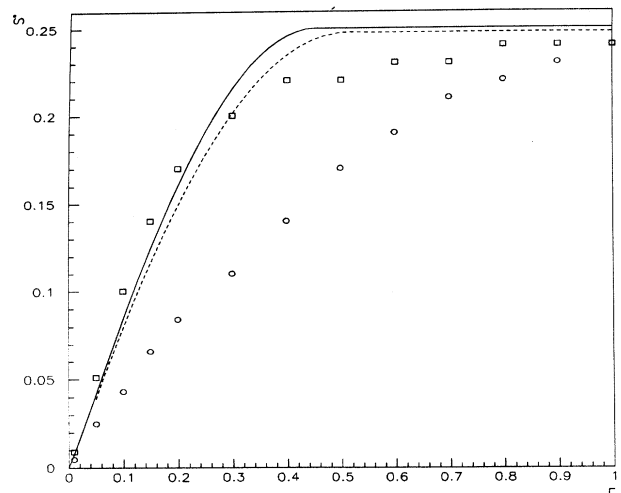


FIG. 4. Minimum QMN action S^* against Γ . The dotted line is from the Hamiltonian method.

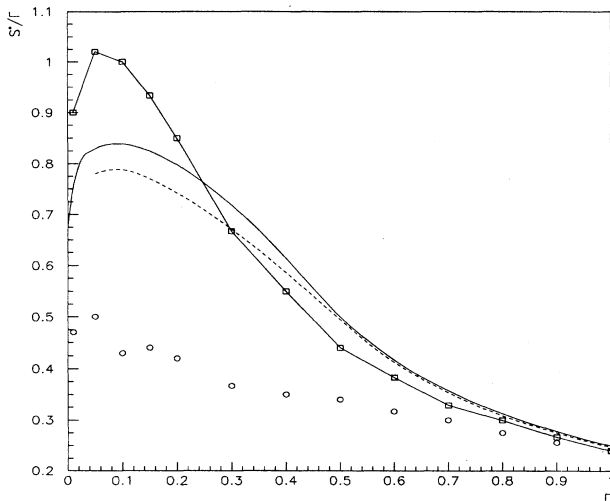


FIG. 5. Minimum QMN action S^*/Γ against Γ . The dotted line is from the Hamiltonian method.

Γ and exists independently of the value of Γ . For $\Gamma > \Gamma_c$ it is the global minimum; however, for $\Gamma < \Gamma_c$ one finds that the optimum path from -1 to 0 bifurcates. In this case this white-noise-type path ceases to be a local minimum and it is the oscillatory-type path which becomes a local minimum. The existence of these latter paths is not obvious when solving Hamilton's equations numerically; a very thorough search in phase space is required to find them. This situation is common in a system such as this with several degrees of freedom: the existence of caustics and focusing gives rise to bifurcations in optimal paths [7], which makes the prediction of the correct action difficult.

An obvious extension of this work is investigate the driving of the underdamped Langevin equation (20) by QMN $\xi(t)$ given by (37). We might expect that driving an equation such as this with harmonic noise such as QMN, we would find a problem that is inherently unstable with oscillatory solutions. This is indeed the case,

and the problem has to be solved using time as an independent variable and by use of a multiple shooting technique. Another added problem is the introduction of two more coordinates, since the Lagrangian now has fourth-order time derivatives. Though this does not cause any further instabilities, it does add to the complexity of the problem and further complicates finding the required solution. We shall not pursue this extension any further, since it does not introduce any novel features.

V. CONCLUSION

The Hamiltonian formalism has proved effective for obtaining results for stochastic systems governed by complicated differential equations. It has allowed us to understand why optimum paths take on particular forms. It also indicates that bifurcations related to caustics and focusing singularities appear as general features of systems governed by colored noise (even those with only one degree of freedom) and not just those with white noise and more than one degree of freedom. The Hamiltonian formalism is the natural one in which to investigate and understand these singularities systematically. We have also shown that the technique of multiple shooting, though slower than relaxation and less convergent, has allowed us to study regions which have so far been elusive and has opened up the solution of these instanton paths in terms of the original (x, t) variables. This could be useful when investigating time-dependent Lagrangians or more complex oscillatory problems. We now feel that the structure and general features of optimal paths are better understood, and that as a consequence the weak-noise evaluation of escape rates and the stationary probability distribution for many stochastic processes is now becoming more straightforward.

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