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COMMENT

On path integrals and stationary probability distributions for stochastic systems

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Abstract. The calculation of the stationary probability distribution for a particle subject to random noise using path-integral methods has been recently discussed in a paper by Rattray and McKane. We wish to point out that this calculation is incorrect, and that the proper analysis avoids some puzzling features of the results presented in the above paper.

In section 2 of their paper, Rattray and McKane [1] consider the calculation of the stationary probability distribution for monostable potentials using steepest descents. We wish to re-examine their approach to this problem, as their results—formally similar to expressions given by other authors—do not yield the correct answer when applied to a simple problem.

Following [1], we consider the problem defined by the Langevin equation

$$\dot{x} = -V'(x) + \xi(t) \tag{1}$$

and we restrict ourselves to white noise for simplicity (coloured noise may be handled using the same methods to be discussed below):

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

The probability of finding the particle at x at time $t=T$, given that it started out at x_0 at time $t=0$ may be expressed as a path integral:

$$P(x, T|x_0, 0) = \int_{x(0)=x_0}^{x(T)=x} \mathrm{D}x\, J[x] \exp(-S[x]/D) \tag{3}$$

where the action is given by

$$S[x] = \frac{1}{4}\int_0^T \mathrm{d}t\, (\dot{x} + V'(x))^2 \tag{4}$$

and the Jacobian $J[x]$ may take different forms depending on the convention adopted to define the path integral. In order to make comparison with the developments in [1] easier—and to be able to use the rules of conventional calculus—we choose

$$J[x]=\exp\left(\frac{1}{2}\int_0^T \mathrm{d}t V''(x)\right). \tag{5}$$

We now seek to evaluate the stationary probability distribution

$$P(x)=\lim_{T\to\infty} P(x, T|x_0, 0) \tag{6}$$

for small D using the method of steepest descents. Setting the first variation of the action (4) equal to zero leads to

$$\dot{x}_c=\pm V'(x_c). \tag{7}$$

Since $S[x]\geqslant 0$, it is clear that the positive sign gives a maximum of the action: the dominant contribution to the integral in (3) must come from the negative sign, regardless of whether we are interested in the 'uphill path beginning at a local minimum' [1] or not. From the mathematical point of view, the fact that the positive sign in (7) is the wrong choice for the method of steepest descents will be reflected in the appearance of negative eigenvalues of the operator associated with the second functional derivative of the action (except for linear and quadratic potentials). From the physical point of view, it would be odd indeed if a vanishingly small noise were capable of effecting the discontinuous change from the negative sign in the deterministic version of equation (1), to a positive sign for infinitesimal D.

For $\dot{x}_c=-V'(x_c)$ the action vanishes: it is therefore seemingly impossible to obtain the Boltzmann factor if we use the negative sign in (7). A careful handling of the boundary conditions shows, however, that this is only an apparent difficulty. Let us compute the path integral in (3) by expanding around the solution with the negative sign. Write

$$x(t)=x_c(t)+f(t)+y(t) \tag{8}$$

where $\dot{x}_c=-V'(x_c)$, $y(t)$ satisfies the usual boundary conditions for Gaussian fluctuations, $y(0)=y(T)=0$, and $f(t)$ is necessary to accommodate the fact that one may impose only one condition on x_c, while the integration variable $x(t)$ is subject to two conditions: $x(0)=x_0$ and $x(T)=x$. If we set $x_c(0)=x_0$, it is clear that we should require $f(0)=0$ and $f(T)=x-x_c(T)$; $f(t)$ itself will be determined below.

Replacing (8) in the action (4) gives, to order $y(t)^2$:

$$S[x]=\frac{1}{4}f(\dot{f}+V''f)|_0^T+\frac{1}{4}\int_0^T f\left(-\frac{\mathrm{d}}{\mathrm{d}t}+V''\right)(\dot{f}+V''f)\,\mathrm{d}t$$

$$+\frac{1}{2}\int_0^T y\left(-\frac{\mathrm{d}}{\mathrm{d}t}+V''\right)(\dot{f}+V''f)\,\mathrm{d}t+\frac{1}{4}\int_0^T(\dot{y}+V''y)^2\,\mathrm{d}t \tag{9}$$

from where we see that a convenient choice for $f(t)$ would satisfy

$$\left(-\frac{\mathrm{d}}{\mathrm{d}t}+V''\right)(\dot{f}+V''f)=0. \tag{10}$$

It is easy to verify that the solution to equation (10), with the stated boundary condition on $f(t)$, is

$$f(t)=[x-x_c(T)]\left\{\dot{x}_c(t)\int_0^t \dot{x}_c^{-2}(t')\,\mathrm{d}t'\right\}\left\{\dot{x}_c(T)\int_0^T \dot{x}_c^{-2}(t')\,\mathrm{d}t'\right\}^{-1}. \tag{11}$$

Substituting in (9) we find, after an integration by parts in the last term

$$\begin{aligned} S[x]&=\frac{1}{4}[x-x_c(T)]^2\left\{\dot{x}_c^2(T)\int_0^T \dot{x}_c^{-2}(t')\,\mathrm{d}t'\right\}^{-1}+\frac{1}{4}\int_0^T y\left(-\frac{\mathrm{d}}{\mathrm{d}t}+V''\right)\left(\frac{\mathrm{d}}{\mathrm{d}t}+V''\right)y\,\mathrm{d}t \\ &\equiv S_1+S_2[y]. \end{aligned} \tag{12}$$

Thus, in the small-D limit the method of steepest descents yields

$$P(x,T|x_0,0)\approx J[x_c]\exp(-S_1/D)\int_{y(0)=0}^{y(T)=0}\mathrm{D}y\exp(-S_2[y]/D). \tag{13}$$

The remaining path integral may be calculated by standard methods [2–4], with the result

$$\int_{y(0)=0}^{y(T)=0}\mathrm{D}y\exp(-S_2[y]/D)=\left\{4\pi D\dot{x}_c(0)\dot{x}_c(T)\int_0^T \dot{x}_c^{-2}(t)\,\mathrm{d}t\right\}^{-1/2}. \tag{14}$$

For the Jacobian we have

$$J[x_c]=\exp\left(\frac{1}{2}\int_0^T \mathrm{d}t V''(x_c)\right)=\exp\left(-\frac{1}{2}\int_0^T \mathrm{d}t\ddot{x}_c/\dot{x}_c\right)=\{\dot{x}_c(0)/\dot{x}_c(T)\}^{1/2}. \tag{15}$$

Thus

$$P(x,T|x_0,0)\approx\left\{4\pi D\dot{x}_c^2(T)\int_0^T \dot{x}_c^{-2}(t)\,\mathrm{d}t\right\}^{-1/2}\exp(-S_1/D). \tag{16}$$

To see that (16) does indeed tend to the correct limit as $T\to\infty$, we now assume for simplicity that the potential has a minimum at $\bar{x}_c$, for which $V(\bar{x}_c)=0$. The 'classical' path $x_c(t)$ will then be driven to this minimum for long times, and therefore $\dot{x}_c(t)\to 0$ as $T\to\infty$. This means that the integrals in (16) are dominated by times $t\approx T$; since

$$\dot{x}_c=-V'(x_c)\approx -V''(\bar{x}_c)(x_c-\bar{x}_c)\equiv -k(x_c-\bar{x}_c) \tag{17}$$

for $t\approx T$, we have $\dot{x}_c(t)\propto \mathrm{e}^{-kt}$, $k>0$, for $t\to\infty$. Hence

$$\int_0^T \dot{x}_c^{-2}(t)\,\mathrm{d}t\approx\{2k\dot{x}_c^2(T)\}^{-1} \tag{18}$$

and (16) has the limit

$$P(x)\approx(k/2\pi D)^{1/2}\exp\{-k(x-\bar{x}_c)^2/2D\}. \tag{19}$$

To the order used in our approximations (see the comment after equation (21) in [1]), $V(x)\approx\frac{1}{2}k(x-\bar{x}_c)^2$, so

$$P(x)\approx\{V''(\bar{x}_c)/2\pi D\}^{1/2}\exp\{-V(x)/D\} \tag{20}$$

which is the expected Boltzmann form.

A simple test of our approach is provided by a quadratic potential. The path integral can be done in closed form, and the answer compared with well-known calculations using other methods [5]. For $V(x)=\frac{1}{2}kx^2$, (16) is no longer an approximation, but the exact result. Since $x_c(t)=x_0\,e^{-kt}$, we find

$$\dot{x}_c^2(T)\int_0^T \dot{x}_c^{-2}(t)\,dt=\frac{1}{2k}\{1-\exp(-2kT)\} \tag{21}$$

and the probability is

$$P(x,T|x_0,0)=\left\{\frac{2\pi D}{k}(1-\exp(-2kT))\right\}^{-1/2}\exp\left\{-\frac{k}{2D}\frac{(x-x_0\exp(-kT))^2}{1-\exp(-2kT)}\right\}. \tag{22}$$

This is the correct expression, but it cannot be obtained from the equations in [1].

As a final remark we should mention a very interesting paper by Weiss [6], who took advantage of the fact that one may explicitly 'factor out' the irreversibility in the path integral [7]. One is left with a modified functional integral which may be handled using the familiar instanton method of ordinary quantum mechanics. Even though his approach is different from ours, it may be verified that his equations reproduce results like (22) above.

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