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Short First-Passage Times

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For diffusion in a monotonic potential field the probability distribution of first-passage times is computed in the limit of short times. The relation to the familiar long-time regime is pointed out.

KEY WORDS: Diffusion; first-passage time.

1. FORMULATION OF THE PROBLEM

Consider an overdamped particle diffusing in a one-dimensional potential well. The probability density $P(x, t)$ is governed by the equation

$$\frac{\partial P}{\partial t}=\frac{\partial}{\partial x} U'(x)P+\theta\frac{\partial^2 P}{\partial x^2} \qquad (x>0) \tag{1}$$

At $x=0$ we take a reflecting boundary (see Fig. 1)

$$U'P+\theta\frac{\partial P}{\partial x}=0 \qquad (x=0, \quad \text{all } t) \tag{2}$$

In order to find the probability distribution of the first-passage time at $x=L$ when starting at some $x_0>0$, one has to solve (1) in the interval $0<x<L$ with condition (2) and

$$P(L, t)=0, \qquad P(x, 0)=\delta(x-x_0) \tag{3}$$

The first-passage time distribution is then identical to the probability flow through L,

$$f(t\,|\,x_0)=-\theta\left[\frac{\partial P(x, t)}{\partial x}\right]_{x=L} \tag{4}$$

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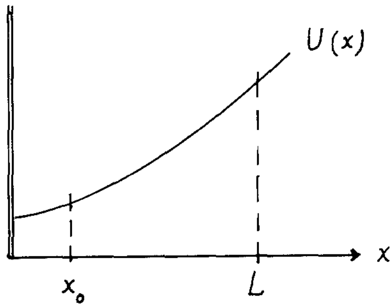

Fig. 1. The interval in which the diffusion takes place.

We assume throughout $U'(x) > 0$ for $0 \leqslant x \leqslant L$. Then for small θ the *mean* first-passage time will be very long, as it involves the Arrhenius factor. For the present case the result is known,[1]

$$\begin{aligned}\tau &= \frac{1}{\theta} \int_0^L e^{U(x)/\theta}\, dx \int_0^x e^{-U(x')/\theta}\, dx' \\ &= \theta [U'(0)\, U'(L)]^{-1} \exp\left[- \frac{U(L) - U(0)}{\theta} \right] \end{aligned} \tag{5}$$

This average corresponds to an exponential term $e^{-t/\tau}$ in the distribution f. We are not concerned with the effort spent on computing τ for more general cases.[2,3]

We are concerned with the behavior of $f(t \mid x_0)$ at *small* values of t. The principal motivation is the nucleation problem.[4] As a concrete example, consider a large volume containing a supersaturated vapor. In order for the condensation to start, a nucleus has to form somewhere; this requires that a potential barrier (or rather a free energy barrier) is surmounted. As soon as this has been achieved somewhere in the volume the whole vapor condenses well-nigh instantaneously. Although it is unlikely for any given nucleus that it overcomes its barrier in a short time, it is not unlikely that this happens somewhere in the volume and that thereby the condensation is triggered. To compute that probability, one needs the short-time behavior of $f(t \mid x_0)$.

An additional motivation is that in the case of stochastic resonance, if the biasing field is strong, the time to overcome the barrier may become short; but this case has not been studied.

2. THE DISTRIBUTION $f(t|x)$ EXPRESSED AS AN INTEGRAL

It is convenient, though not strictly necessary, to cast (1) into an eigenvalue problem of Schrödinger type by setting[5]

$$P(x, t) = e^{-\lambda t} e^{-U(x)/2\theta}\, \Phi(x) \tag{6}$$

so that $\Phi(x)$ obeys

$$\theta \frac{d^2\Phi}{dx^2} + \left[\lambda - \frac{U'(x)^2}{4\theta} + \frac{U''(x)}{2}\right]\Phi = 0 \tag{7}$$

$$[\tfrac{1}{2}U'\Phi + \theta\Phi']_{x=0} = 0, \qquad \Phi(L) = 0 \tag{8}$$

Moreover, I multiply with θ and set $\lambda\theta = \mu$:

$$\theta^2\Phi'' + [\mu - W(x)]\,\Phi = 0 \tag{9}$$

$$W(x) = \tfrac{1}{4}U'(x)^2 - \tfrac{1}{2}\theta U''(x) \tag{10}$$

Define $\Phi(x, \mu)$ for any μ as that solution of the second-order equation (9) that is given by the initial conditions

$$\Phi(0, \mu) = 1, \qquad \Phi'(0, \mu) = -U'(0)/2\theta \tag{11}$$

For each value of x this function $\Phi(x, \mu)$ is analytic in the entire complex μ-plane.[6] The eigenvalues μ_n are the solutions of

$$\Phi(L, \mu) = 0 \tag{12}$$

The eigenfunctions $\Phi(L, \mu_n)$ are orthogonal, complete, but not normalized, so that

$$\sum_n \frac{\Phi(x_0, \mu_n)\,\Phi(x, \mu_n)}{\int_0^L \Phi(x', \mu_n)^2\, dx'} = \delta(x - x_0) \tag{13}$$

The desired solution of (1)–(3) may then be written

$$P(x, t) = e^{-[U(x) - U(x_0)]/2\theta} \sum_n e^{-\mu_n t/\theta} \frac{\Phi(x_0, \mu_n)\,\Phi(x, \mu_n)}{\int_0^L \Phi(x', \mu_n)^2\, dx'} \tag{14}$$

According to (4), one now has

$$f(t\,|\,x_0) = -\theta e^{-[U(L) - U(x_0)]/2\theta} \sum_n e^{-\mu_n t/\theta} \frac{\Phi(x_0, \mu_n)\,\Phi(L, \mu_n)}{\int_0^L \Phi(x', \mu_n)^2\, dx'} \tag{15}$$

This expression may be rewritten with the use of the following identity. Differentiate (9) with respect to μ, to be indicated by a subscript μ,

$$\theta^2 \Phi''_\mu + [\mu - W(x)]\,\Phi_\mu + \Phi = 0 \tag{16}$$

Multiply (9) with Φ_μ and (16) with Φ, subtract, and integrate:

$$\theta^2[\Phi_\mu \Phi' - \Phi\Phi'_\mu]_0^L = \int_0^L \Phi^2\,dx \tag{17}$$

On the left, the boundary $x=0$ does not contribute because $\Phi_\mu(0) = \Phi'_\mu(0) = 0$ according to (11). If one inserts $\mu = \mu_n$, one also has $\Phi(L, \mu_n) = 0$, so that one is left with the identity

$$\theta^2 \Phi_\mu(L, \mu_n)\,\Phi'(L, \mu_n) = \int_0^L \Phi(x, \mu_n)^2\,dx \tag{18}$$

Substitution of this identity in (15) gives

$$f(t\,|\,x_0) = \frac{-1}{\theta}\, e^{-[U(L) - U(x_0)]/2\theta} \sum_n e^{-\mu_n t/\theta}\, \frac{\Phi(x_0, \mu_n)}{\Phi_\mu(L, \mu_n)} \tag{19}$$

This may be written in the form (see Fig. 2)

$$f(t\,|\,x_0) = \frac{-1}{2\pi i\theta}\, e^{-U(L) - U(x_0)/2\theta} \int_C e^{-\mu t/\theta}\, \frac{\Phi(x_0, \mu)}{\Phi(L, \mu)}\, d\mu \tag{20}$$

where C is the contour in the complex μ-plane surrounding all μ_n. This remarkable integral expression for $f(t\,|\,x_0)$ is exact and will serve as the starting point of our calculation.

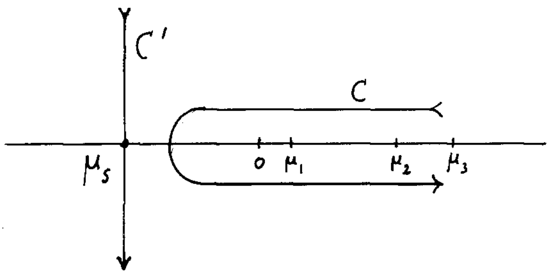

Fig. 2. The integration contour around the poles.

3. APPROXIMATIONS

When μ lies on C one knows that $W(x)-\mu\neq 0$, so that for small θ the WKB method may be used:

$$\Phi(x,\mu)=A\exp\left[\frac{1}{\theta}K(x)\right]+B\exp\left[-\frac{1}{\theta}K(x)\right] \tag{21}$$

$$K(x,\mu)=\int_0^x [W(x')-\mu]^{1/2}\,dx' \tag{22}$$

This neglects terms of order θ in the exponent. Also a factor

$$[W(x)-\mu]^{-1/4}=[K'(x,\mu)]^{-1/2} \tag{23}$$

ought to have been included in (21), but it does not affect the result of this section and has been omitted for simplicity. We also use (for typographical reason) $\beta=1/\theta$, so that β is a large parameter. The integration constants are determined by the initial conditions (11),

$$A=\frac{1}{2}-\frac{U'(0)}{4K'(0,\mu)},\qquad B=\frac{1}{2}+\frac{U'(0)}{4K'(0,\mu)} \tag{24}$$

For small θ, large β, and $x_0>0$ the first term of (21) dominates and one may omit the second one. Using this approximation in (20), one finds

$$f(t\,|\,x_0)=\frac{-\beta}{2\pi i}\exp\left\{-\frac{1}{2}\beta[U(L)-U(0)]\right\}$$
$$\times\int_C \exp\{-\beta[\mu t-K(x_0,\mu)+K(L,\mu)]\}\,d\mu \tag{25}$$

In order to apply the saddle point method I write $h(\mu)$ for the quantity $[\cdots]$. The saddle point μ_s is the solution of

$$h'(\mu)=t-\frac{1}{2}\int_{x_0}^{L}\frac{dx'}{[W(x')-\mu]^{1/2}}=0 \tag{26}$$

The only possibility is that μ is real and less than $m\equiv\mathrm{Min}\,W(x)$. It is then seen from Fig. 3 that there is one μ_s for every $t>0$. Moreover, $\mu_s\to-\infty$ as $t\to 0$, so that approximately for small t,

$$t\approx\frac{L-x_0}{2(-\mu_s)^{1/2}},\qquad \mu_s\approx-\left(\frac{L-x_0}{2t}\right)^2 \tag{27}$$

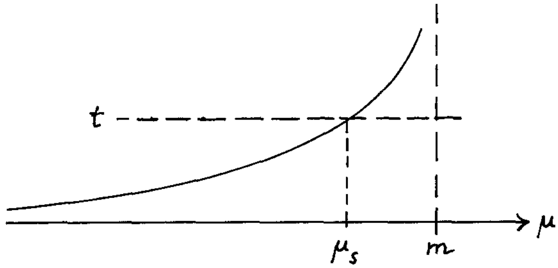

Fig. 3. Solving Eq. (26) for the saddle point.

The second derivative is

$$h''(\mu_s) = -\frac{1}{4}\int_{x_0}^{L} \frac{dx'}{[W(x') - \mu_s]^{3/2}} \approx \frac{-2t^3}{(L-x_0)^2} \tag{28}$$

If we now open up C into a vertical line through μ_s we obtain for (25)

$$f(t\,|\,x_0) = \frac{\beta}{2\pi}\exp\left\{-\frac{1}{2}\beta[U(L) - U(0)]\right\}$$
$$\times \exp[-\beta h(\mu_s)]\left[\frac{2\pi}{\beta h''(\mu_s)}\right]^{1/2} \tag{29}$$

With the same small-time approximation one has

$$h(\mu_s) \approx \mu_s t + (L - x_0)(-\mu_s)^{1/2} = \frac{(L-x_0)^2}{4t} \tag{30}$$

The final result is

$$f(t\,|\,x_0) = Ct^{-3/2}\exp\left[-\frac{(L-x_0)^2}{4\theta t}\right] \tag{31}$$

$$C = \frac{L - x_0}{2(\pi\theta)^{1/2}}\exp\left[-\frac{U(L) - U(x_0)}{2\theta}\right] \tag{32}$$

The saddle point approximation requires that the saddle point μ_s is sufficiently far from the poles; as these are all positive, it means that $|\mu_s|$ must be larger than the width of the peak, which is determined by (28):

$$\left(\frac{L-x_0}{2t}\right)^2 > \left[\frac{1}{\theta}\frac{2t^3}{(L-x_0)^2}\right]^{-1/2} \quad \text{or} \quad \frac{(L-x_0)^2}{\theta t} > 1 \tag{33}$$

Thus (31) applies until t is so large that the exponential is indistinguishable from unity.

4. THE LONG-TIME BEHAVIOR

All eigenvalues μ_n are positive, but some are more positive than others. In particular, the lowest one, μ_1, which determines the long-time behavior of $f(t|x_0)$, is very close to zero. To evaluate it, we insert the WKB expression (21), (22) into the eigenvalue equation (12) and obtain

$$e^{-2\beta K(L,\mu_1)} = -\frac{A}{B} = \frac{\frac{1}{2}U'(0) - K'(0,\mu_1)}{\frac{1}{2}U'(0) + K'(0,\mu_1)} \tag{34}$$

The left-hand side is very small and therefore so is the numerator on the right, so that

$$[W(0)-\mu_1]^{1/2} = \tfrac{1}{2}U'(0) - U'(0)\exp[-2\beta K(L,\mu_1)] \tag{35}$$

Squaring, omitting higher orders, and putting $K(L,\mu_1)\approx K(L,0)$, we obtain

$$\begin{aligned}\mu_1 &= U'(0)^2 \exp\left\{-2\beta\int_0^L [W(x)]^{1/2}\,dx\right\}\\ &= U'(0)^2 \exp\left\{-\beta\int_0^L [U' - \theta U''/U']\,dx\right\}\\ &= U'(0)\,U'(L)\exp\{-\beta[U(L)-U(0)]\}\end{aligned} \tag{36}$$

Hence the sum (19) contains the long-lived exponential $\exp(-\mu_1 t/\theta)$ in agreement with (5).

Suppose one begins with a small value of t, for which the result (31) was derived, and allows t to grow. The saddle point μ_s shifts to the right and reaches μ_1 when t equals

$$t_1 = \frac{1}{2}\int_{x_0}^L \frac{dx'}{[W(x')]^{1/2}} \approx \int_{x_0}^L \frac{dx'}{U'(x')} \tag{37}$$

Subsequently $f(t|x_0)$ may be written as a residue of the pole μ_1 plus an integral over a contour C_1 to the right of μ_1. We compute the residue, i.e., the first term of (19).

The numerator $\Phi(x_0,\mu_1)$ is given by (21), but the first term is negligible, as A/B is small according to (34). On the other hand, it is now necessary to reinstate the factor (23), which reduces to $[\frac{1}{2}U'(x)]^{-1/2}$. Hence one finds, using the same algebra as in (36),

$$\begin{aligned}\Phi(x_0,\mu_1) &= [U'(x_0)/U'(0)]^{-1/2} B\exp[-\beta K(x_0,0)]\\ &= \exp\{-\tfrac{1}{2}\beta[U(x_0)-U(0)]\end{aligned} \tag{38}$$

To find the numerator $\Phi_\mu(L, \mu_1)$, one has to differentiate the exponent in (21) with respect to μ, but the resulting terms are exponentially small. In addition, one has to differentiate A and B; this produces one large term, which, including the factor (23), works out to

$$\Phi_\mu(L, \mu_1) = \left[\frac{U'(L)}{U'(0)}\right]^{-1/2} \frac{-U'(0)}{8[K'(0,0)]^3} \exp[\beta K(L, 0)]$$

$$= -[U'(0)\, U'(L)]^{-1} \exp\left\{\frac{1}{2}\beta[U(L) - U(0)]\right\} \tag{39}$$

Substitution of (38) and (39) yields for the first term of (19)

$$f_1(t \mid x_0) = \frac{1}{\theta}\, U'(0)\, U'(L) \exp\left[-\frac{U(L) - U(0)}{\theta}\right] \exp\frac{-s_1 t}{\theta} \tag{40}$$

This is the well-known result obtained from the familiar calculation of the mean first-passage time as in (5).

5. DISCUSSION

If $U = 0$ the diffusion equation (1) can be solved exactly. The result is (31), but also a second term appears, due to particles that are reflected by the boundary at $x = 0$. Such particles are absent here because for them the exponential factor in (32) would be exponentially smaller. It follows that (31) is made up of particles that have never visited the boundary at $x = 0$. Consequently (31) is valid regardless of the boundary condition (2). Incidentally, one sees from this why it was necessary to require $U'(x) > 0$ and also $x_0 > 0$. The case $x_0 = 0$ can easily be treated by including the second term in (21).

The integral of (31) is

$$\int_0^\infty f(t \mid x_0)\, dt = \exp\left[-\frac{U(L) - U(x_0)}{2\theta}\right] \tag{41}$$

This is the total probability for the first passage to take place within the short-time regime. Actually it is only an upper bound for the probability, since the integral ought to be extended up to the time given by (33) rather than up to ∞. The integral of the long-time regime (40) equals unity, again with a correction for the short times. Thus the total probability for a short first-passage time is small, of the order (41): almost all first passages occur after a long time comparable to (5). The former never experience the bottom of the well, the latter move about in the well for a long time and forget their starting point x_0. Between both regimes there is a transition region not covered by the calculations.

Our condition $U(x) > 0$ for $0 \leqslant x \leqslant L$ can be relaxed so as to permit a rounded barrier top and a flat well bottom. The short-time result (31), (32) remains valid, but the long-time formula must be amended in the familiar way.[1]

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