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LETTER TO THE EDITOR

Kramers time in bistable potentials

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Abstract. Diffusion in a general bistable potential governed by the Fokker-Planck equation is studied for large t. A simple variational calculation yields a lower bound for the Kramer's time. The method (using a supersymmetric pair of Hamiltonians) applies immediately to diffusion in a potential with a large number of minima and to bistable potentials in higher dimension characterised by a most probable escape path.

Diffusion in a bistable has often been studied since it is the prototype of problems which involve an approach to equilibrium. In its simplest one-dimensional form one considers a potential $U(x)$ with two minima at $x = a$ and $x = b$, separated by a maximum at $x = 0$ (figure 1). A particle starts out at the unstable point $x = 0$ and feels a small random force in addition to the force derived from the potential. It is conventional to treat the high-viscosity limit, where the equation of motion becomes

$$\dot{x} = -\frac{dU}{dx} + f(t) \tag{1}$$

$f(t)$ being the random noise, specified by the correlation

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

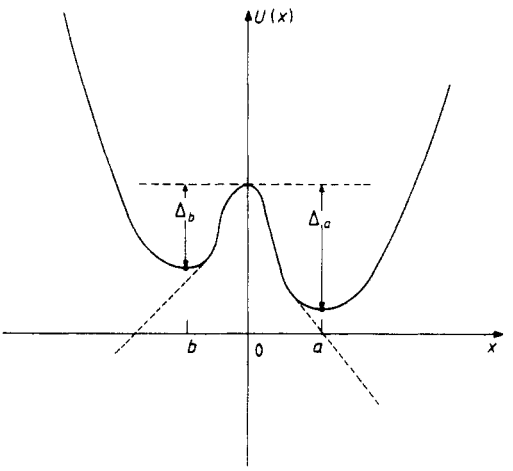

Figure 1. The general bistable potential in one dimension. The function $\phi(x)$ in the trial wavefunction follows $U(x)$ close to the two minima and then joins smoothly to the linearly decreasing functions as shown by the broken lines.

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The approach to equilibrium is best described in terms of the Fokker-Planck equation for the probability distribution $p(x, t)$,

$$\frac{\partial p}{\partial t}=\frac{\partial}{\partial x}\left(p\frac{\partial U}{\partial x}\right)+\varepsilon\frac{\partial^2 p}{\partial x^2}. \tag{3}$$

The equilibrium solution is

$$p_{eq}(x)=\mathrm{d}(-U/\varepsilon). \tag{4}$$

To find the time-dependent solution of (3), one makes the substitution

$$p(x, t)=\exp(-U/2\varepsilon)\phi(x, t) \tag{5}$$

and obtains for $\phi(x, t)$ the Schrödinger-like equation

$$-\varepsilon\frac{\partial\phi}{\partial t}=-\varepsilon^2\frac{\partial^2\phi}{\partial x^2}+V(x)\phi \tag{6}$$

where

$$V(x)=\tfrac{1}{4}U'(x)^2-\tfrac{1}{2}\varepsilon U''(x) \tag{7}$$

and finds

$$\phi(x, t)=\sum_n a_n\exp(-\lambda_n t)\phi_n(x)$$

where $\phi_n(x)$ are the complete set of eigenstates of the Hamiltonian $H=-\varepsilon^2\partial^2/\partial x^2+V(x)$, with

$$H\phi_n(x)=\lambda_n\phi_n(x). \tag{8}$$

The Hamiltonian of (6) is positive semi-definite with lowest eigenvalue zero with the wavefunction

$$\phi_0(x)=A\exp(-U(x)/2\varepsilon).$$

Thus,

$$p(x, t)=A\exp(-U(x)/\varepsilon)+\sum_{n=1}^{\infty}a_n\exp(-\lambda_n t)\phi_n(x)\exp(-U(x)/2\varepsilon). \tag{9}$$

Three timescales can now be identified in the problem:

(i) the initial period when the probability distribution of $t=0$ (sharp peak at $x=0$) begins to spread out due to diffusion;

(ii) the intermediate time regime of Suzuki [1], where the broadening central peak begins to split into two side peaks corresponding to the minima of $U(x)$ at $x=a$ and $x=b$;

(iii) the final time regime of Kramers [2], where the system is close to equilibrium but can make occasional large fluctuations due to the noise.

Here we are interested in the final regime. The time to attain true equilibrium is now controlled by the lowest excited state of (8), namely the eigenvalue λ_1. An analytic technique that yields λ_1 is the WKB method (note that λ_1 is exponentially close to the ground-state energy, zero, and differs from it only because of the tunnelling in the three-well problem posed by the potential of (7)) and a formidable calculation by Caroli *et al* [3] yields the answer

$$\lambda_1=C\varepsilon[(|U_0''|U_a'')^{1/2}\exp(-\Delta_a/\varepsilon)+(|U_0''|U_b'')^{1/2}\exp(-\Delta_b/\varepsilon)] \tag{10}$$

where C is a constant (equal to $(2\pi)^{-1}$ in the WKB calculation of Caroli *et al* and

$$\Delta_{a,b} = U_0 - U_{a,b} \tag{11}$$

with U_n denoting the value of $U(x)$ at $x = n$. The problem of finding λ_1 by calculating the splitting of the lowest state of H due to tunnelling can be converted to the determination of the ground state of the supersymmetric partner of H. A variational calculation will now yield an upper limit to the value of λ_1. Here, we show that for an arbitrary $U(x)$, one can obtain λ_1 from a variational calculation and always cast the answer in the form of (10). Our best variational wavefunction yields $C = \frac{1}{6}e^{3/2}(6\pi)^{-1/2} \simeq 0.17$. One can now extend the calculation to a potential $U(x)$ which has N minima and establish that the eigenvalue λ_1 vanishes as $N \to \infty$, i.e. in the limit when $U(x)$ becomes periodic. Consequently, supersymmetry is broken when $U(x)$ is periodic and the classical particle can diffuse, i.e. $\langle x^2 \rangle$ increases with time. Thus for the transition from localised to extended states in the classical problem supersymmetry is the symmetry that is broken in the equivalent quantum problem. We also treat the two-dimensional bistable potential and in the case that the minima are connected by a most probable escape path [5] establish that the lowest eigenvalue λ_1 is given by

$$\lambda_1 = C\varepsilon[(|U_0''|U_a'')^{1/2}(W_a/W_0)^{1/2}\exp(-\Delta_a/\varepsilon) + (|U_0''|U_b'')^{1/2}(W_b/W_0)^{1/2}\exp(-\Delta_b/\varepsilon)] \tag{12}$$

where the constant C is once again $\frac{1}{6}e^{3/2}(6\pi)^{-1/2}$.

To establish (10) for the one-dimensional potential $U(x)$ (see figure 1), we proceed as follows.

As noted by Bernstein and Brown [4], λ_1 is obtained as the ground-state energy of the supergrammetric partner of the Hamiltonian of (6), where the potential $V(x)$ is replaced by $\tilde{V}(x) = -\frac{1}{4}U'(x)^2 + \frac{1}{2}\varepsilon U''(x)$. Thus, one requires the ground-state energy of $H = -\varepsilon^2 d^2/dx^2 + \tilde{V}(x)$. This is to be obtained by a variational calculation. We observe that $\exp(U(x)/2\varepsilon)$ is an eigenstate of the above Hamiltonian with eigenvalue zero. However, this function is not normalisable. Hence we choose the trial function $\exp(\phi(x)/2\varepsilon)$, where

(i) $\phi(x) = U(x)$ for $b(1-\alpha_b\varepsilon^{1/2}) < x < a(1-\alpha_a\varepsilon^{1/2})$

(ii) $\phi(x) = U(a-a\varepsilon^{1/2}\alpha_a) + U'(a-a\alpha_a\varepsilon^{1/2})(x - a^{+}a\alpha_a\varepsilon^{1/2})$
for $x > a(1-\alpha_a\varepsilon^{1/2})$

(iii) $\phi(x) = U(b-b\varepsilon^{1/2}\alpha_b) + U'(b-b\alpha_b\varepsilon^{1/2})(\dot{x} - b + b\alpha_b\varepsilon^{1/2})$
for $X < b(1-\alpha_b\varepsilon^{1/2})$.

In the above, we have assumed that ε is small and anticipated the distance scale to be $O(\varepsilon^{1/2})$, so that α, the variational parameter, is going to be a number of O(1). Note that the matching occurs near the turning points in the classical region for the corresponding Schrödinger equation. We now need to evaluate the expectation value, $\lambda_1(\alpha)$ as

$$\lambda_1(\alpha) = \frac{\int_{-\infty}^{\infty}\exp(\phi(x)/2\varepsilon)\tilde{H}\exp(\phi(x)/2\varepsilon)\,dx}{\int_{-\infty}^{\infty}\exp(\phi(x)/\varepsilon)\,dx}. \tag{13}$$

The calculation involves the following steps.

(i) Evaluating the normalisation integral, we note that $\phi(x) \simeq U(0) - \frac{1}{2}U''(0)X^2$ for small x and this maximum value of $\phi(x)$ dominates the integral for $\varepsilon \ll 1$. Thus, the normalisation integral is $\exp((U_0/\varepsilon)\sqrt{2\pi\varepsilon/U_0''}$.

(ii) The kinetic energy and potential energy terms cancel completely when $\phi(x) = U(x)$. Thus the integration in the numerator of equation (13) involves integrating from $a(1-\varepsilon^{1/2}\alpha_a)$ to ∞ and from $b(1-\varepsilon^{1/2}\alpha_b)$ to $-\infty$.

(iii) In the range of integration discussed in (ii) about $x = a$ and $x = b$, it is sufficient to approximate the potential $U(x)$ by a quadratic expression for $\varepsilon \ll 1$. Terms like $U(a - a\varepsilon^{1/2}\alpha_a)$ and $U'(a - a\varepsilon^{1/2}\alpha_a)$ need to be expanded to $O(\varepsilon)$ to obtain the leading term, and it should be noted that $U'(a) = U'(b) = 0$.

We thus obtain $\lambda_1(\alpha)$. Minimisation with respect to $\alpha_{a,b}$ leads to the conditions that

$$a^2\alpha_a^2 U''(a) = b^2\alpha_b^2 U''(b) = 3 \tag{14}$$

thus establishing (10) with $C = \frac{1}{2}e^{3/2}(6\pi)^{-1/2}$. For the class of potentials treated by Bernstein and Brown [4] our result agrees exactly with theirs.

We take up the two-dimensional problem with the $U(x, y)$ having the form shown in figure 2. Our assumption about $U(x, y)$ is going to be that made by Caroli *et al* [5]—namely that there exists a most probable escape path (the instanton trajectory) which we take to be the x axis in this case and about this escape path $U(x, y)$ can be expanded as

$$U(x, y) = U(x) + \tfrac{1}{2}W(x)y^2 \tag{15}$$

where $U(x)$ is the potential that we have discussed above. The Hamiltonian of (8) is now

$$H = -\varepsilon^2\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + V(x, y) \tag{16}$$

with

$$V(x, y) = \frac{1}{4}\left(\frac{\partial U}{\partial x}\right)^2 + \left(\frac{\partial U}{\partial y}\right)^2 + \frac{\varepsilon}{2}\left(\frac{\partial^2 U}{\partial x^2} + \frac{\partial^2 U}{\partial y^2}\right)$$

The ground state of H is $\exp(-U(x, y)/2\varepsilon)$ and the eigenvalue is zero. As before, we are interested in the first excited state.

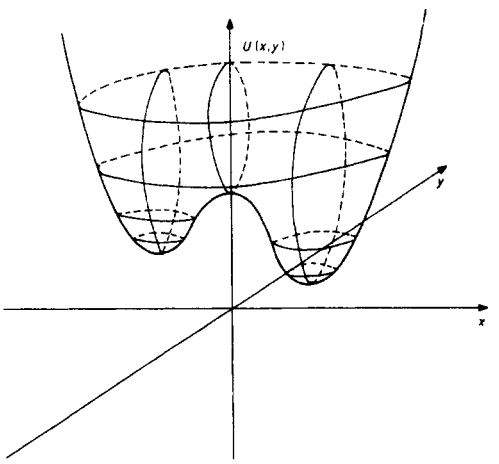

Figure 2. The general bistable potential in two dimensions. The most probable escape path is the x axis.

One notes immediately that the first excited state will involve changes (mainly) in the x direction, retaining the y dependence of the wavefunction as $\exp(-w(x)y^2/2\varepsilon)$ to a good approximation. This 'stiffness' in the y direction suggests a variant of the Born–Oppenheimer approximation where we solve the y-dependent part of the Hamiltonian, treating the x dependence as a parameter. The resulting eigenvalue will be a function of x and will act as an effective potential for the one-dimensional problem in x. Introducing (15) into (16), we find the y-dependent part of the Hamiltonian to be

$$-\varepsilon^2\partial^2/\partial y^2+\tfrac{1}{4}(w^2+U'w'-W'')y^2$$

whose lowest eigenvalue is clearly $\frac{1}{2}\varepsilon\sqrt{w^2+U'w'-\varepsilon w''}$. Noting that w is a slowly varying function, so that w'/w and w''/w are $\ll 1$, we can expand the above expression and write down the Hamiltonian for the x direction problem as

$$\begin{aligned}\mathscr{H} &= -\varepsilon^2\frac{\mathrm{d}^2}{\mathrm{d}x^2}+\frac{U'^2}{4}-\frac{\varepsilon}{2}U''+\varepsilon\frac{U'w'}{4w}-\frac{\varepsilon^2 w''}{4w}\\ &\simeq\left(-\varepsilon\frac{\mathrm{d}}{\mathrm{d}x}+\frac{u'}{2}+\varepsilon\frac{w'}{4w}\right)\left(\varepsilon\frac{\mathrm{d}}{\mathrm{d}x}+\frac{U'}{2}+\varepsilon\frac{w'}{4w}\right)\end{aligned} \tag{17}$$

where, in writing the second line, we have not matched the higher-order term $\varepsilon^2(w'/w)^2$. We require the two lowest eigenvalues of the Hamiltonian of (17) and, in addition, to obtain the first excited state we need the ground state of the supersymmetric partner of H, which is given by

$$\bar{\mathscr{H}}=\left(\varepsilon\frac{\mathrm{d}}{\mathrm{d}x}+\frac{U'}{2}+\frac{w'}{4w}\right)\left(-\varepsilon\frac{\mathrm{d}}{\mathrm{d}x}+\frac{U'}{2}+\frac{w'}{4w}\right). \tag{18}$$

We now take over the variational calculation for the one-dimensional case discussed above. The *only* difference to be noted is that the non-normalisable function which gives zero eigenvalue is now

$$\exp(U(x)/2\varepsilon)\exp\left(\frac{1}{4}\int_0^x\frac{W'(x)}{W(x)}\mathrm{d}x\right).$$

For $\varepsilon\ll 1$, this term yields $\exp[\frac{1}{2}\ln(W(a)/W(0))]$ for the range of integration from $a(1-\alpha_a\varepsilon^{1/2})$ to ∞ and a similar term for the range $b(1-\alpha_b\varepsilon^{1/2})$ to $-\infty$, when one calculates the expectation value. We thus obtain (12). Generalisation to higher (n) dimension is straightforward. There will be $(n-1)$ transverse directions characterised by $(n-1)$ functions $W_j(x)$ and the factor $W(a)/W(0)$ will be replaced by

$$\left(\prod_{j=1}^{n-1}\frac{W_j(a)}{W_j(0)}\right)^{1/2}.$$

Finally, we return to the one-dimensional problem and consider a potential $U_N(x)$ with N minima, with all the minima and intervening maxima of equal height. As $N\to\infty$, the potential passes over to the periodic potential which has been investigated before [6]. It is known that for the periodic potential, the behaviour is diffusive and in the long-time limit the mean-square displacement increases linearly from localised to diffusive behaviour. Proceeding exactly as for the one-dimensional case, we note that in (13), the evaluation of the numerator produces exactly the same answer as before, but the denominator now has $N-1$ ($\simeq N$ for $N\gg 1$) terms (all maxima are equal) and hence the lowest eigenvalue $\lambda_1^{(N)}$ is obtained as $\lambda_1^{(N)}=\lambda_1/N$, where λ_1 is given by (10), the two terms of (10) standing for the two extreme minima of the above

potential. Clearly as $N \to \infty$, the first excited state eigenvalue tends to zero. The ground state becomes degenerate, resulting in the breaking of supersymmetry and transition from localised to diffusive behaviour for $t \to \infty$.

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