

## Escape and Splitting Probabilities in Diffusive and Non-Diffusive Markov Processes

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The  $\mathcal{Q}$ -expansion of the master equation for Markov processes may either lead to a non-diffusive or, under certain conditions, to a diffusive type of approximation. In the first case bistability is defined by the macroscopic equation, in the second case by the properties of the resulting non-linear Fokker-Planck equation. In both cases one may ask for the probability per unit time to flip from one locally stable point to the other, and for the probability that a system starting near the intervening unstable point will go to either one of the two stable points. It is possible to give explicit expressions for these quantities in the case of one-dimensional diffusive systems and in the case of (non-diffusive) one-step processes. The various methods are listed and compared.

### § 1. Two types of master equation

A Markov process  $X(t)$  can be described by its transition probability  $P(x, t|x_0, t_0)$  defined for  $t \geq t_0$ . It obeys the Chapman-Kolmogorov or master equation

$$\frac{\partial P(x, t)}{\partial t} = \int \{W(x|x')P(x', t) - W(x'|x)P(x, t)\} dx',$$

where we have omitted the initial data  $x_0, t_0$ . The jump probability per unit time  $W(x|x')$  from  $x'$  to  $x$  normally contains a parameter  $\mathcal{Q}$  having the property that for large  $\mathcal{Q}$  the fluctuations are relatively small in a certain sense;  $\mathcal{Q}$  is often the size of the system.<sup>1)</sup> Expansion in powers of  $\mathcal{Q}^{-1/2}$  yields first

$$\frac{\partial P(x, t)}{\partial t} = -\frac{\partial}{\partial x} \alpha_{1,0}(x) P(x, t),$$

where  $\alpha_{1,0}$  is the first jump moment taken to lowest order in  $\mathcal{Q}^{-1}$ :

$$\int (x-x')^n W(x|x') dx = \alpha_{n,0}(x') + \mathcal{Q}^{-1} \alpha_{n,1}(x') + \dots$$

In this approximation the master equation reduces therefore to the Liouville equation of the deterministic process

$$\dot{x} = \alpha_{1,0}(x).$$

*This is the macroscopic or phenomenological equation.*

If this macroscopic equation has a single stationary solution obeying  $\alpha_{1,0}(x^{\text{st}}) = 0$  and all other solutions tend towards it, then the higher order terms in the master equation (which describe the fluctuations around the macroscopic solutions) remain small and the  $\Omega$ -expansion can be used for all times  $t > t_0$  (Fig. 1). If, however, there are unstable solutions of the macroscopic equation the fluctuations around them grow in time and the  $\Omega$ -expansion is valid only for a limited initial period. Hence other methods are needed for the case of a bistable equation as in Fig. 2. Various models of systems governed by such a macroscopic equation have been studied in recent years.<sup>2)</sup> We shall call this type I bistability.

A marginal case is  $\alpha_{1,0}(x) \equiv 0$ . Then the macroscopic first order approximation to the master equation vanishes, and the lowest order in the  $\Omega$ -expansion is the nonlinear Fokker-Planck equation

$$\frac{\partial P(x, t)}{\partial t} = \Omega^{-1} \left[ -\frac{\partial}{\partial x} \alpha_{1,1}(x) P + \frac{1}{2} \frac{\partial^2}{\partial x^2} \alpha_{2,0}(x) P \right].$$

Thus *the familiar diffusion approximation to the master equation follows from the  $\Omega$ -expansion only in this marginal case.*<sup>3)</sup> A physical example of this diffusion case is the migration of electrons in a semiconductor, subject to an external electrostatic potential  $U(x)$

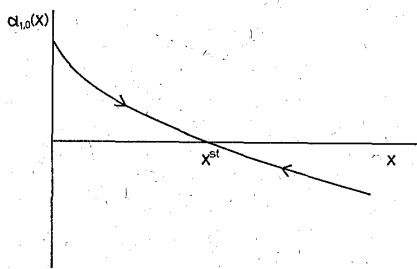


Fig. 1.(a)

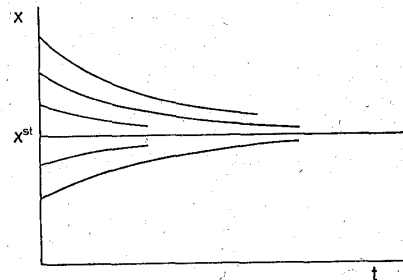


Fig. 1.(b)

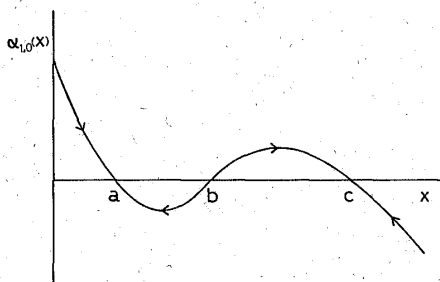


Fig. 2.(a)

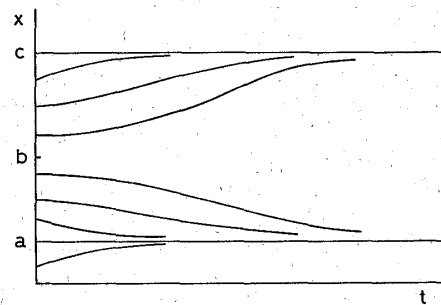


Fig. 2.(b)

$$\frac{\partial P(x, t)}{\partial t} = \mu \frac{\partial}{\partial x} U'(x) P + D \frac{\partial^2 P}{\partial x^2}.$$

$\mu$  is the mobility,  $D$  the diffusion constant, and  $D = \mu kT/e$ . Here bistability can occur when  $U$  has the form of Fig. 3; this will be called type II bistability.<sup>15)</sup>

The fundamental difference between both cases should be clear. Type II bistability is not determined by the macroscopic equation (which is simply  $\dot{x} = 0$ ). The sole cause for  $P$  to vary is provided by the fluctuations. A deterministic equation can only be extracted by manipulating *another* parameter than  $\Omega$ , namely by setting  $D = 0$  (that is,  $T = 0$ ). The fact that the resulting equation

$$\dot{x} = -\mu U'(x)$$

is related to the equilibrium distribution

$$P^{\text{eq}}(x) = C \exp[-\mu U(x)/D] = C \exp[-eU(x)/kT]$$

is the basis of extensive studies.<sup>4)</sup> This relation, however, is only true for master equations of the diffusion type with constant  $D$ - and of course for the equivalent Langevin equation

$$\begin{aligned} \dot{x} &= -\mu U'(x) + L(t), \\ \langle L(t) \rangle &= 0, \quad \langle L(t) L(t') \rangle = 2D\delta(t-t'). \end{aligned}$$

## § 2. The escape probability for bistable diffusion

We shall discuss bistability first for the diffusion type master equation because differential equations are more familiar than integral equations. In particular we take the example mentioned above with  $\mu = 1$ ,

$$\frac{\partial P(x, t)}{\partial t} = \frac{\partial}{\partial x} U'(x) P + D \frac{\partial^2 P}{\partial x^2},$$

where  $U(x)$  is given in Fig. 3, which for convenience is taken symmetric around  $x = 0$ . (Appendix B.) There are two main questions one may ask about such a system, which we shall label by  $(\tau)$  and  $(\pi)$ .

$(\tau)$  The *escape probability*  $1/\tau_{ca}$ , that is, the probability per unit time for a system that is in local or metastable equilibrium near  $a$  to be carried across the potential barrier into  $c$  by fluctuations.

$(\pi)$  The *splitting probability*  $\pi_c(x_0)$ , that is, the probability that a system initially at  $x_0$  will end up at  $c$ , or  $\pi_a(x_0) = 1 - \pi_c(x_0)$  to end up at  $a$ .

Both questions are only well-defined provided that the potential barrier is

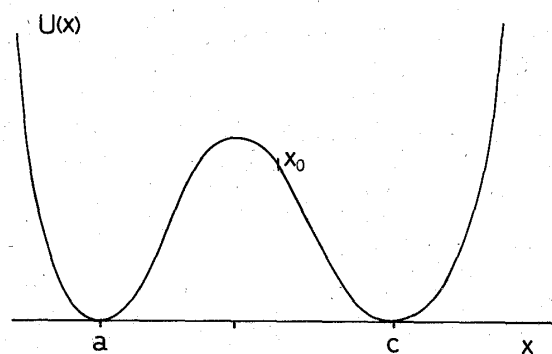


Fig. 3.

high, so that the metastable equilibrium distributions near  $a$  and  $c$  are long-lived. Then there is a clear separation between the short time scale on which these local equilibria are reached and the long time scale on which they exchange probability between them so as to reach the ultimate equilibrium  $P^{\text{eq}}$ . We shall *not* be concerned with the critical phenomena that occur when the barrier is lowered down to zero.

*Both the escape probability and the splitting probability can be computed without solving the master equation.* The only approximations needed are based on the assumption that the potential barrier is high. The resulting margin of error is therefore of the same order as the uncertainty in the very definition of the quantities  $\tau$  and  $\pi$ . We now list the methods that have been used to compute  $\tau_{ca}$ .

( $\tau 1$ ) Kramers<sup>5)</sup> computed the escape probability by an ingenious manipulation of the diffusion equation resulting in

$$\tau_{ca} = \sqrt{\frac{2}{DU''(a)}} \int_a^c \exp\left[\frac{U(x) - U(a)}{D}\right] dx.$$

This is the general result, which only requires that  $\tau_{ca}$  is much larger than the characteristic time for reaching local equilibrium in each potential valley, i.e.,

$$\tau_{ca} \gg \tau_{aa} \sim \{U''(a)\}^{-1}.$$

If, in addition, the potential maximum at  $b$  is sharp one has

$$\tau_{ca} \simeq \frac{2\pi}{\sqrt{U''(a)|U''(b)|}} \exp\left[\frac{U(b) - U(a)}{D}\right].$$

The exponential factor dominates and had already been guessed by Arrhenius in 1889. This simple formula, however, involves the additional assumption that  $D$  is small; in fact it is the first term of the asymptotic expansion of the above general result for  $D \rightarrow 0$ . The same result has been obtained in a different way by Griffiths, Wang and Langer.<sup>6)</sup>

( $\tau_2$ ) Consider the *first-passage problem*: When a system starts at  $a$ , what is the probability distribution of the time at which it first passes through  $c$ ? The answer requires the solution of the same diffusion equation with initial condition  $P(x, 0) = \delta(x - a)$ , but in the range  $-\infty < x < c$  and with an absorbing boundary at  $x = c$ , that is,  $P(c, t) = 0$ . To find the escape probability, however, one only needs the *mean* first passage time from  $a$  to  $c$ :

$$\tau_{ca} = \int_0^\infty t \left[ -D \frac{\partial P}{\partial x} \right]_c dt = \int_{-\infty}^c dx \int_0^\infty P(x, t) dt \equiv \int_{-\infty}^c dx \bar{P}(x).$$

Thus *one only needs the time integrated probability density*  $\bar{P}(x)$ . An equation for it is obtained by integrating the master equation over  $0 < t < \infty$ :

$$-\delta(x - a) = \frac{d}{dx} U'(x) \bar{P}(x) + D \frac{d^2 \bar{P}(x)}{dx^2},$$

which can readily be solved for  $-\infty < x < c$  with  $\bar{P}(c) = 0$ . The resulting  $\tau_{ca}$  is the same as the general form of the Kramers result.

( $\tau_3$ ) The original diffusion equation is equivalent to the *eigenvalue problem*

$$-\lambda P(x) = \frac{d}{dx} U'(x) P(x) + D \frac{d^2 P(x)}{dx^2}$$

with normalizability condition

$$\int_{-\infty}^\infty e^{U(x)/D} \{P(x)\}^2 dx < \infty.$$

The discussion of this eigenvalue problem is facilitated by the fact that it can be translated into the more familiar language of a Schrödinger equation<sup>7),8)</sup>

$$\phi''(x) + \{E - V(x)\} \phi(x) = 0$$

with the following dictionary. If  $E_n$ ,  $\phi_n$  are the eigenvalues and normalized eigenfunctions of the Schrödinger equation;  $\lambda_n$ ,  $P_n$  those of the diffusion equation:

$$U(x) = -D \log \phi_0(x),$$

$$\lambda_n = D(E_n - E_0),$$

$$P_n(x) = \phi_0(x) \phi_n(x).$$

In order that  $U(x)$  has the bistable form of Fig. 3 one must also have a bistable  $V(x)$ . One then knows from elementary quantum mechanics that  $\phi_0(x)$  is symmetric,  $\phi_1(x)$  antisymmetric, and  $E_1 - E_0$  very small, while  $E_2$ ,  $E_3$ , ... are much higher. The very small time factor  $\lambda_1 = D(E_1 - E_0)$  can be identified with the escape probability

$$\lambda_1 = \tau_{ca} + \tau_{ac} = 2\tau_{ca}.$$

It is shown in Appendix A that this agrees with Kramers' result.

### § 3. The splitting probability

Let  $x_0$  be small and positive and let  $P(x, t|x_0, 0)$  be the solution of the diffusion equation which at  $t=0$  reduces to  $\delta(x-x_0)$ . On a time scale much less than  $\tau_{ca}$  it will split into two peaks around  $a$  and  $c$  respectively with total probabilities  $\pi_a(x_0)$  and  $\pi_c(x_0)$ . Our aim is to compute them without solving the full diffusion equation.

( $\pi 1$ ) The following plausible approach has tempted several authors. Supposing  $x_0$  small one approximates  $U(x)$  near the origin  $b$  by a parabola

$$U(x) = U(b) - \frac{1}{2}|U''(b)|x^2.$$

With this linearization the diffusion equation can be solved explicitly. The resulting  $P(x, t|x_0, 0)$  should be a good approximation to the actual one during some initial period of order  $|U''(b)|^{-1}$ . After this period the probability flow across the top should be negligible so that the separation into  $\pi_a$  and  $\pi_c$  has been completed. If desired, the further evolution of  $P(x, t|x_0, 0)$  can subsequently be computed in each potential valley separately, for instance by means of the  $\Omega$ -expansion.

Unfortunately the explicit calculation for a solvable model has shown that this method leads to an incorrect result.<sup>8)</sup> This can be understood by realizing that the solution of the linearized diffusion equation is a (rapidly shifting and broadening) Gaussian, so that it never leads to a clear separation into  $\pi_a$  and  $\pi_c$ . The emergence of two separate peaks<sup>9)</sup> in the distribution is a consequence of the nonlinearity of  $U'(x)$ .

( $\pi 2$ ) In analogy with ( $\tau 2$ ) one may formulate the following first passage problem: Starting at  $x_0$  what is the probability for passing through  $a$  before reaching  $c$  and vice versa? Let  $P(x, t)$  be the solution of the diffusion equation in the range  $a < x < c$  with the absorbing boundary conditions  $P(a, t) = P(c, t) = 0$ . Then

$$\pi_a = \int_0^\infty \left[ D \frac{\partial P}{\partial x} \right]_a dt, \quad \pi_c = \int_0^\infty \left[ -D \frac{\partial P}{\partial x} \right]_c dt.$$

Again it is sufficient to know the time integrated solution  $\bar{P}(x)$ , which can be found explicitly. The result is

$$\pi_a = \frac{1}{2} - \int_b^{x_0} e^{U(x')/D} dx' / \int_a^c e^{U(x')/D} dx'.$$

If one replaces the integrand in the denominator by its peak and supposes  $x_0$  small this reduces to

$$\pi_a = \frac{1}{2} - \frac{1}{2} \operatorname{erf}[x_0 \sqrt{|U''(b)|/2D}].$$

This is the same result as obtained by the linearization procedure ( $\pi 1$ ) and is numerically incorrect, because one cannot replace every integral by a Gaussian. That is only correct if in addition one takes the limit  $D \rightarrow 0$ , as is done by Suzuki.<sup>10</sup> To compute a splitting probability, however, one must then simultaneously let  $x_0$  tend to zero, because for fixed  $x_0$  in the limit  $D \rightarrow 0$  one obviously has  $\pi_a = 0$ ,  $\pi_c = 1$ .

( $\pi 3$ ) The eigenfunction expansion mentioned under ( $\tau 3$ ) yields

$$P(x, t | x_0, 0) = \phi_0(x)^2 + \frac{\phi_1(x_0)}{\phi_0(x_0)} \phi_0(x) \phi_1(x) e^{-D(E_1 - E_0)t} \\ + \sum_{n=2}^{\infty} \frac{\phi_n(x_0)}{\phi_0(x_0)} \phi_0(x) \phi_n(x) e^{-D(E_n - E_0)t}.$$

The terms with  $n \geq 2$  damp out on the short time scale while the one with  $n=1$  disappears very slowly. Hence in the time interval

$$[D(E_2 - E_0)]^{-1} \ll t \ll [D(E_1 - E_0)]^{-1}$$

one has

$$\pi_a = \int_{-\infty}^b P(x, t | x_0, 0) dx = \frac{1}{2} - \frac{1}{2} \frac{\phi_1(x_0)}{\phi_0(x_0)}.$$

It is shown in Appendix A that this is the same as found above, assuming always that the barrier is high.

#### § 4. Non-diffusive Markov processes

Of all Markov processes which are governed by a master equation that is not of diffusion type we select the special subclass of one-step or birth-and-death processes

$$\dot{P}(n, t) = r(n+1)P(n+1, t) - r(n)P(n, t) \\ + g(n-1)P(n-1, t) - g(n)P(n, t).$$

The two coefficient functions  $g(n)$  and  $r(n)$  for generation and recombination are supposed to be smooth functions of  $n$ . The equilibrium distribution is given for  $n > 0$  by

$$P^{\text{eq}}(n) = \frac{g(n-1)g(n-2)\cdots g(0)}{r(n)r(n-1)\cdots r(1)} P^{\text{eq}}(0),$$

and similarly for  $n < 0$ . If one chooses to write this as  $P^{\text{eq}}(n) = \exp[-U(n)]$  one has

$$U(n) = \sum_{\nu=1}^n \{\log r(\nu) - \log g(\nu-1)\} + \text{const.}$$

The macroscopic equation is

$$\dot{n} = \alpha_1(n) = g(n) - r(n).$$

(If  $g$  and  $r$  contain higher order of  $\Omega^{-1}$  they should be omitted in this equation, but we shall here ignore this complication.) If one chooses to write this equation as  $\dot{n} = -dV/dn$  one has

$$V(n) = \sum_{\nu=1}^n \{r(\nu) - g(\nu)\} + \text{const.}$$

Thus, in contrast with the diffusion type *the potential  $V$  of the macroscopic equation is not the same as the "free energy"  $U$  defined by  $P^{\text{eq}}$* . Rather one can show

$$\exp\left(\frac{dU}{dn}\right) - 1 = \frac{1}{g(n)} \frac{dV(n)}{dn}.$$

As the maxima and minima of  $U$  and  $V$  coincide either one may be used to define bistability (in section 1 we used  $V$ ).

For bistable one-step processes it is again possible to give explicit expressions for  $\tau$  and  $\pi$  without solving the master equation. In fact, despite the profound physical difference between Markov processes of types I and II, the mathematical analogy between one-step processes and diffusion processes is sufficiently close for similar methods to be applicable.

( $\tau 1$ ) The Kramers method carries over to one-step processes<sup>11)</sup> in the form

$$\tau_{ca} = \frac{1}{2} \sum_a^c \frac{1}{r(n) P^{\text{eq}}(n)}.$$

Here  $a$  and  $c$  are values of  $n$  at or near the two stability points; their precise values are irrelevant because the main contribution comes from the neighborhood of where  $P^{\text{eq}}(n)$  is very small. The normalization factor of  $P^{\text{eq}}$  corresponds to the square root in Kramers' expression for  $\tau_{ca}$  in the diffusion case.

( $\tau 2$ ) The method with an absorbing boundary or first-passage method also carries over and gives the same result.

( $\tau 3$ ) More interesting is that the normal mode method also carries over to one-step processes and that the eigenvalue equation can again be translated into a Schrödinger-like difference equation. It is therefore also possible to construct a special case that can be solved explicitly, and thereby investigate



the influence of the step size on the escape probability. This work is in progress but no precise results are yet available.

As to the splitting probability, the linearizing approximation ( $\pi 1$ ) is again wrong. The absorbing boundary method ( $\pi 2$ ) for one-step processes has been used by Oppenheim, Shuler and Weiss,<sup>12)</sup> but they solved the resulting first passage problem in a different way. The application of the eigenfunction method ( $\pi 3$ ) has not yet been completed.

### § 5. Further problems

Although the diffusion equation is mathematically simpler than a difference equation and enjoys great popularity, it should be borne in mind that it has no divine right. Kolmogorov's derivation is based on the Lindeberg condition, which corresponds to the unphysical picture of a random process as a succession of infinitely many infinitely small jumps.<sup>13)</sup> The nonlinear Fokker-Planck equation is merely an approximation, which in terms of the  $\Omega$ -expansion only applies to the marginal class of Markov processes for which  $\alpha_{1,0}=0$ . It is therefore important to extend the computation of  $\tau$  and  $\pi$  to more realistic master equations such as that for one-step processes. However, for more general master equations involving steps of more than one size no explicit expressions for  $\tau$  and  $\pi$  are available and much more elaborate methods are needed.<sup>14)</sup>

In the multidimensional case, i.e., when  $x$  stands for several variables, a much richer variety of stability situations is possible. For instance the macroscopic equations could have one stable point and one limit cycle, and one may ask for the probability per unit time that it flips from the one into the other regime. For this problem the Kramers ( $\tau 1$ ) does not seem to work any more. The absorbing boundary method ( $\tau 2$ ) is possible in principle, but the first-passage problem can no longer be solved explicitly for the general case. As to ( $\tau 3$ ): It is of course possible to expand formally in normal modes, but this does not lead to general explicit answers either.

### Appendix A

To find the connection between the eigenfunction method and the other results one needs approximate expressions for  $E_1 - E_0$  and for  $\phi_1(x)$  that are valid when the potential barrier is high. Setting  $\phi_1(x) = \phi_0 \{1 - g(x)\}$  one has

$$\phi_0 g'' + 2\phi_0' g' - (E_1 - E_0)\phi_0 = (E_1 - E_0)\phi_0 g.$$

As  $g$  is small for most of the interval  $x > 0$  neglect the right-hand side. Then

$$\phi_0^2(x) g'(x) = - (E_1 - E_0) \int_x^\infty \phi_0^2(x') dx',$$

$$g(x) = -(E_1 - E_0) \int_0^x \frac{dx'}{\phi_0^2(x')} \int_{x'}^\infty \phi_0^2(x'') dx'' + A.$$

As  $g(0) = 1$  one has  $A = 1$  and hence (see also Ref. 7))

$$\begin{aligned} (E_1 - E_0)^{-1} &= \int_0^\infty \frac{dx'}{\phi_0^2(x')} \int_{x'}^\infty \phi_0^2(x'') dx'' \\ &= \int_0^\infty e^{\bar{U}(x')/D} dx' \int_{x'}^\infty e^{-\bar{U}(x'')/D} dx'' \\ &\simeq \int_0^c e^{\bar{U}(x')/D} dx' \sqrt{\frac{2\pi D}{U''(a)}} \end{aligned}$$

in agreement with Kramers' general result for  $\tau_{ca}$ . In addition one obtains

$$\begin{aligned} \pi_a &= \frac{1}{2} g(x_0) = \frac{1}{2} - \frac{1}{2} (E_1 - E_0) \int_0^{x_0} e^{\bar{U}(x')/D} dx' \int_{x'}^\infty e^{-\bar{U}(x'')/D} dx'' \\ &\simeq \frac{1}{2} - \frac{1}{2} \int_0^{x_0} e^{\bar{U}(x')/D} dx' / \int_0^c e^{\bar{U}(x')/D} dx', \end{aligned}$$

in agreement with the result found under  $(\pi 2)$ .

## Appendix B

Consider diffusion in an asymmetrical potential  $U(x)$ , Fig. 4(a). The equilibrium distribution  $P^{\text{eq}}(x) = C e^{-U(x)}$  consists of a large peak at  $c$  and a small one at  $a$  (Fig. 4(b)). For the relative probabilities in each one easily finds

$$\frac{\pi_a^{\text{eq}}}{\pi_c^{\text{eq}}} = \sqrt{\frac{U''(c)}{U''(a)}} e^{-[U(a) - U(c)]/D}.$$

In the limit  $D \rightarrow 0$  the small one disappears, unless both minima of  $U$  have

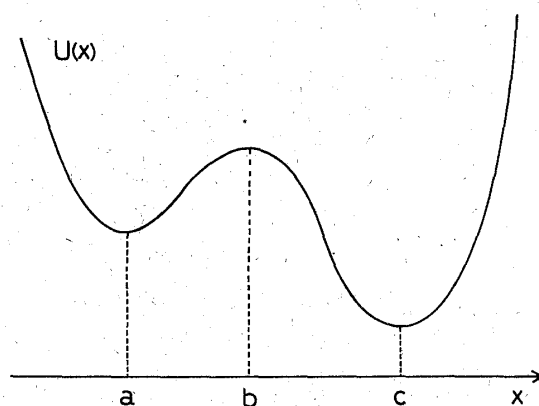


Fig. 4.(a)

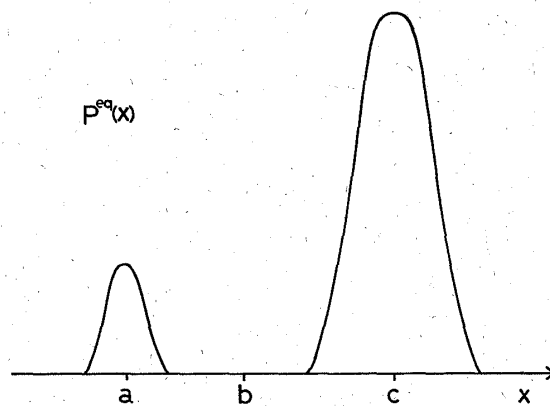


Fig. 4.(b)

equal height. The same is true in the case of a one-step process in the limit  $\Omega \rightarrow \infty$ , because the free energy  $U(n) = -\log P^{\text{eq}}$  contains a factor  $\Omega$ . What has this fact to do with "relative stability"?

If the master equation refers to a chemical reaction in an open system having two stable stationary states  $a$  and  $c$ , one may imagine a vessel in which both regimes occur simultaneously in different parts of the volume. One then expects that the volume in which the "more stable" regime  $c$  occurs grows at the expense of the other.<sup>10)</sup> Only if both minima have equal height is co-existence possible. Our simple one-step master equation, however, does not describe any spatial dependence but refers to homogeneous systems alone. It cannot therefore really serve to describe such situations, but a reasonable short-cut seems possible. The putting together of both regime in one vessel may be viewed as opening up a loophole in the barrier, through which the states  $a$  and  $c$  can exchange probability other than by a giant fluctuation over the top. The very long escape times  $\tau_{ca}$  and  $\tau_{ac}$  are thereby artificially shortened. Otherwise the same picture holds and we conclude that the state  $c$  with the lowest minimum of  $U$  will drive out state  $a$ , provided that  $D \ll U(a) - U(c)$  (for the diffusion case), or  $U(a) - U(c) \gg 1$  (for the one-step process).

The escape probabilities for an asymmetric bistable system can be computed in the same way as for the symmetric case and the results are

$$\begin{aligned} \frac{\tau_{ca}}{\pi_a^{\text{eq}}} &= \frac{\tau_{ac}}{\pi_c^{\text{eq}}} = \int_a^c \frac{dx}{P^{\text{eq}}(x)} \quad (\text{diffusion case}) \\ &= \sum_a^c \frac{1}{r(n) P^{\text{eq}}(n)} \quad (\text{one-step process}). \end{aligned}$$

Note that detailed balance holds. Note also that the ratio of  $\tau_{ca}$  and  $\tau_{ac}$  determines the relative stability of  $a$  and  $c$ , but only because of the factors  $\pi_a$  and  $\pi_c$ ; the integral (or the sum) is not needed. To compute  $\tau_{ca}$  and  $\tau_{ac}$  in order to find the relative stability of  $a$  and  $c$  would be circuitous.

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### Discussion

**H. Haken:** I am a little bit doubtful if one may discuss coexistence of phases in extended media by means of "short-circuit" between the two peaks of the distribution function. Such a coupling by diffusion terms could lead to new kinds of distributions including spatial patterns.

**N. G. van Kampen:** Of course one cannot hope to describe spatial patterns in the framework of these one-variable equations. The only purpose of my "short-circuit" is to simulate within this framework the effect of putting two phases together into a vessel, in order to be able to talk about the "relative stability" mentioned by Prof. Ross in his talk.

**J. Ross:** There is an analogy to the question of relative stability of two stable stationary states as posed by the arrangement in which two semi-infinite regions, one for each state, are placed in contact. The relative stability is determined by the velocity of the soliton produced as one phase eats up another. The analogy is that of two phases, say, liquid and vapor, in equilibrium with each other and arranged as just described. If the temperature is lowered then the liquid-vapor boundary moves, as a soliton, to destroy the vapor phase; if the temperature is raised the reverse occurs. If we assume a cubic in density (van der Waals) and add diffusion, then the resulting "reaction-diffusion" equation can be solved analytically (E. Montroll). No nucleation process occurs here.

**H. Haken:** I think that the results you mention depend on specific cases. For instance, for two (local) state variables with different diffusion coefficients, the original "local" distribution can be distributed appreciably leading to spatial patterns and not to a homogeneous phase.

**N. G. van Kampen:** My variable  $x$  or  $n$  represented the overall density or concentration of a substance in a strongly stirred system. Of course no spatial

variations can survive the stirring. In order to describe those one has to start with a master equation for the probability  $P\{n(r)\}$  in the space of density functions  $n(r)$ . It would be not just a multivariate, but an infinitely-variable problem. That can be done, but is of course much more complicated. In particular, it is no longer possible to find the explicit expressions that were the subject of this lecture.

**G. Nicolis:** 1) I would like to mention an important result from the theory of non-linear partial differential equations. It asserts that in systems containing a single variable and subject to natural boundary conditions, one cannot have stable time-independent but space-dependent solutions. The only issue left is either a uniform profile or a wavefront propagating in the medium.

2) From the theory of diffusion processes, we know that a continuous Markov process satisfies a non-linear Fokker-Planck equation if the Kolmogorov conditions on the transition probability are satisfied. Would you comment on the distinction between "Type I" and "Type II" diffusion processes made in your talk in the light of this result?

**N. G. van Kampen:** There is a wide-spread misconception that every Markov process whose values can vary in a continuous range must obey the (nonlinear) Fokker-Planck equation. The reason is that physicists are overawed by the rigorous derivation of that equation by Kolmogorov. Actually his proof is based on a very strong premiss, which (in physical terms) states that every change is caused by infinitely many infinitely small jumps. For simple physical processes it can be shown explicitly that this condition is not obeyed, e.g., for the Brownian particle. There is reason to believe that it is never realized in physics, since all fluctuations are caused by the particle nature of matter and therefore consist of jumps of the order of an atomic mass or of an electron charge, etc. The Fokker-Planck equation is therefore at best an approximation, but should therefore also be derived by a systematic approximation method. That is just what the  $\mathcal{Q}$ -expansion is, and it turns out that this expansion does indeed lead to the nonlinear Fokker-Planck equation, but only in the special case that  $\alpha_{1,0}(x) \equiv 0$ .

**R. Kubo:** The problem is a stationary state. There is a source and two absorbing walls. And calculate flows at the wall to obtain the splitting.

**N. G. van Kampen:** Quite. The master equation with absorbing boundaries, after it has been integrated over time, can be visualized as a stationary probability flow originating at  $x_0$  and splitting up in a left and right flow, with ratios  $\pi_a$  and  $\pi_c$ .