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SINGULAR PERTURBATION METHODS IN STOCHASTIC DIFFERENTIAL EQUATIONS OF MATHEMATICAL PHYSICS*

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Abstract. Stochastic differential equations are used as models for various physical phenomena, such as chemical reactions, atomic migration in crystals, thermal fluctuations in electrical networks, noisy signals in radio transmission, etc. First passage times of solutions of such equations from certain domains and the distribution of the exit points are computed from the solutions of singularly perturbed elliptic boundary value problems. Physical interpretation of these quantities is given. Applications in communication theory and in reliability of structures are shown.

1. Introduction. Since Einstein gave the mathematical theory of the Brownian motion and applied it to explain molecular diffusion, a large body of scientific work has been done on the theory and applications of this discovery. The applications range over such diverse scientific areas as molecular and atomic physics, chemical kinetics, solid state diffusion phenomena, stability of mechanical structures, electrical network and filtering theory, wave propagation in random media, population genetics and many other branches of the natural and social sciences. The most prominent work in the early stages of stochastic differential equations was done by Einstein, Langevin, Smoluchowski, Kramers and their contemporaries. This work was summarized in Chandrasekhar's survey paper (Chandrasekhar [6]).

The mathematical theory of stochastic differential equations was developed in the last thirty years and several texts on this subject have appeared recently e.g. (Gihman and Skorohod [13]). Significant progress was made with the discovery of the partial differential equations for the distribution and moments of first passage times for solutions of stochastic equations. The Itô calculus in particular gave the theory of stochastic differential equations in bounded domains an important tool. The behavior of solutions at boundaries determines boundary conditions for solutions of appropriate parabolic and elliptic partial differential equations. The close relationship between first passage times and boundary value problems for partial differential equations makes the powerful methods of asymptotic analysis of partial differential equations available for the study of such first passage problems. The absence of adequate theory or adequate computational methods for solving first passage problems severely limited the scope of modeling physical phenomena by stochastic differential equations. Alternative methods were devised to overcome this difficulty. Such is the case e.g., of the transition state method for the computation of chemical reaction rates and for the description of diffusion phenomena in solids. The need for first passage theory arises in situations where a particle is trapped in a potential well while random forces tend to "liberate" it by pushing it over the potential barrier. The purpose of this paper is to present sources of stochastic differential equations in mathematical physics and to present the new singular perturbations methods that were recently developed for the solutions of the appropriate first passage problems.

2. Langevin's equation and Brownian motion. The chaotic perpetual motion of a Brownian particle is the result of its collisions with the molecules of the surrounding fluid. The molecular collisions of a Brownian particle occur in very rapid succession and their number is tremendous. Thus a Brownian particle (e.g. colloidal gold particles of

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radius 50 $\mu\,\mu$) will suffer about 10^{21} collisions per second if immersed in liquid under normal conditions. This frequency is so high that the small changes in the particle's path caused by each single impact are too fine to be discerned by the observer. Thus the exact path of the particle cannot be followed in any detail but has to be described statistically. The force acting on a Brownian particle consists of a hydrodynamical drag and a force due to individual collisions with the particles of the surrounding fluid. The principal assumptions concerning the second, fluctuating force $\mathbf{f}(t)$ (per unit mass) are the following: (i) $\mathbf{f}(t)$ is statistically independent of the velocity $\mathbf{v}(t)$ of the particle, (ii) the variations of $\mathbf{f}(t)$ are much more frequent than the variations in $\mathbf{v}(t)$, and (iii) the average of $\mathbf{f}(t)$ is zero. Newton's equations of motion are then given by

$$d\mathbf{v}(t)/dt = -\beta\mathbf{v}(t)+\mathbf{f}(t) \tag{2.1}$$

where β is the drag coefficient. Equation (2.1) is called *Langevin's equation.* The statistical properties of $\mathbf{f}(t)$ can be deduced from this equation by matching its solution with known physical laws. The solution of the stochastic differential equation (2.1) determines the transition probability density $p(\mathbf{v}, t, \mathbf{v}_0)$ of the random process $\mathbf{v}(t)$ i.e. a function $p(\mathbf{v}, t, \mathbf{v}_0)$ such that

$$P(\mathbf{v}(t)\in A \mid \mathbf{v}(0)=\mathbf{v}_0) = \int_A p(\mathbf{v}, t, \mathbf{v}_0)\, d\mathbf{v}$$

where $A \subset R^3$. Assuming that the initial velocity $\mathbf{v}_0$ is given we must have

$$p(\mathbf{v}, t, \mathbf{v}_0)\to\delta(\mathbf{v}-\mathbf{v}_0) \quad \text{as } t\to 0$$

where δ is Dirac's function. Further, we know from statistical physics that the density $p(\mathbf{v}, t, \mathbf{v}_0)$ must approach the Maxwellian density for the temperature T of the surrounding medium, independently of $\mathbf{v}_0$ as $t\to\infty$. Hence

$$p(\mathbf{v}, t, \mathbf{v}_0)\to\left(\frac{m}{2\pi kT}\right)^{3/2}\exp\left(-m|\mathbf{v}|^2/kT\right) \tag{2.2}$$

where m is the mass of the Brownian particle and k is Boltzman's constant. This demand on $p(\mathbf{v}, t, \mathbf{v}_0)$ requires $\mathbf{f}(t)$ in turn to have certain statistical properties. The formal solution (2.1) is given by

$$\mathbf{v}(t) = \mathbf{v}_0\, e^{-\beta t} + \int_0^t e^{-\beta(t-s)}\mathbf{f}(s)\, ds \tag{2.3}$$

provided the integral exists. Consequently the statistical properties of the integral must be the same as those of the difference $\mathbf{v}(t)-\mathbf{v}_0\, e^{-\beta t}$. Since

$$\mathbf{v}(t)-\mathbf{v}_0\, e^{-\beta t}\approx\mathbf{v}(t)$$

for large t, the integral must have in the limit a Gaussian density. Writing the integral as a finite (Riemann) sum

$$\int_0^t e^{-\beta(t-s)}\mathbf{f}(s)\, ds \approx e^{-\beta t}\sum_n e^{\beta n\Delta t}\mathbf{f}(n\,\Delta t)\,\Delta t \equiv e^{-\beta t}\sum_n e^{\beta n\Delta t}\,\Delta\mathbf{b}_n,$$

where $\Delta\mathbf{b}_n = \mathbf{f}(n\,\Delta t)\,\Delta t$, we obtain for large t

$$\mathbf{v}\approx\sum_n e^{\beta(n\Delta t-t)}\,\Delta\mathbf{b}_n. \tag{2.4}$$

The random variables $\Delta\mathbf{b}_n$ express the random accelerations suffered by a Brownian

particle in the time interval $(n\,\Delta t, (n+1)\,\Delta t)$. Thus we may assume that the variables $\Delta\mathbf{b}_n$ are statistically independent of each other, since the successive collisions are completely chaotic. We shall assume that the time intervals Δt are large compared to the average period of a single fluctuation of $\mathbf{f}(t)$. The period of fluctuation of $\mathbf{f}(t)$ is of the order of the time between successive collisions between the Brownian particle and the molecules of the surrounding fluid; in a liquid this is generally of the order of 10^{-21} sec. Accordingly, each acceleration $\Delta\mathbf{b}_n$ is the result of many collisions, so that we may assume that all $\Delta\mathbf{b}_n$ have the same statistical properties (Chandrasekhar [6]). If we choose therefore $\Delta\mathbf{b}_n$ to be zero mean Gaussian variables the $\mathbf{v}(t)$ will be Gaussian as required in (2.2). To compute the variance of $\Delta\mathbf{b}_n$ we set

$$E|\Delta\mathbf{b}_n|^2 = 2q\,\Delta t$$

and using (2.4) we obtain

$$E|\mathbf{v}|^2 = \sum_n 2q\,\Delta t\, e^{2\beta(n\Delta t - t)} \to 2q\int_0^t e^{2\beta(s-t)}\,ds$$

$$= \frac{q}{\beta}(1 - e^{-2\beta t}) \quad \text{as } \Delta t \to 0.$$

On the other hand we have

$$E|\mathbf{v}|^2 \to \frac{kT}{m} \quad \text{as } t \to \infty$$

by (2.2); hence

$$q = \beta kT/m. \tag{2.5}$$

Let $\mathbf{x}(t)$ be the displacement of the Brownian particle. Then

$$\mathbf{x}(t) = \mathbf{x}_0 + \int_0^t \mathbf{v}(s)\,ds. \tag{2.6}$$

Substituting (2.3) in (2.6) we obtain

$$\mathbf{x}(t) = \mathbf{x} + \int_0^t \left[\mathbf{v}_0\, e^{-\beta s} + e^{-\beta s}\int_0^s e^{\beta u}\mathbf{f}(u)\,du\right] ds.$$

Using integration by parts we get

$$\begin{aligned}\mathbf{x}(t) - \mathbf{x}_0 - \mathbf{v}_0(1 - e^{-\beta t})/\beta &= -e^{-\beta t}\int_0^t e^{\beta s}\mathbf{f}(s)\,ds/\beta \\ &\quad + \int_0^t \mathbf{f}(s)\,ds/\beta \equiv \int_0^t g(s)\mathbf{f}(s)\,ds.\end{aligned} \tag{2.7}$$

Where $g(s) = (1 - e^{\beta(s-t)})/\beta$. Using a finite sum approximation to the integral again we conclude that the variable

$$\mathbf{x}(t) - \mathbf{x}_0 - \mathbf{v}_0(1 - e^{-\beta t})/\beta$$

is a zero mean Gaussian variable with variance

$$\sigma^2 = \int_0^t g^2(s)\,ds = \frac{1}{2\beta^2}(2\beta t - 3 + 4\,e^{-\beta t} - e^{-2\beta t}). \tag{2.8}$$

Hence the probability density of $\mathbf{x}(t)$ is given by

$$p(\mathbf{x}, t, \mathbf{x}_0, \mathbf{v}_0) = \{m\beta^2/[2\pi kT(2\beta t - 3 + 4\, e^{-\beta t} - e^{-2\beta t})]\}^{3/2} \cdot \exp\left\{-\frac{m\beta^2|\mathbf{x}-\mathbf{x}_0-\mathbf{v}_0(1-e^{-\beta t})/\beta|^2}{[2kT(2\beta t - 3 + 4\, e^{-\beta t} - e^{-2\beta t})]}\right\}. \tag{2.9}$$

For large t we have

$$p(\mathbf{x}, t, \mathbf{x}_0, \mathbf{v}_0) \approx (4\pi Dt)^{-3/2} \exp\left(-|\mathbf{x}-\mathbf{x}_0|^2/(4Dt)\right), \tag{2.10}$$

where

$$D = kT/(m\beta). \tag{2.11}$$

Using Stokes' formula for the drag coefficient we get $\beta = 6\pi a\eta$ where a is the radius of the Brownian particle and η is the viscosity coefficient of the surrounding fluid. It follows that $p(\mathbf{x}, t, \mathbf{x}_0, \mathbf{v}_0)$ becomes independent of $\mathbf{v}_0$ and satisfies the diffusion equation

$$\partial p/\partial t = D\, \Delta p$$

with the diffusion coefficient D given by (2.11). This is Einstein's result (cf. Einstein [10]). Note that the pair $(\mathbf{x}(t), \mathbf{v}(t))$ is Markovian but $\mathbf{x}(t)$ is not. For large β the joint transition density of $(\mathbf{x}(t), \mathbf{v}(t))$ splits into a product of two densities, so $\mathbf{x}(t)$ and $\mathbf{v}(t)$ converge to Markovian processes as $\beta \to \infty$ (cf. Chandrasekhar [6], Feller [11], Kac [18]). We can define now the Brownian motion $\mathbf{x}(t)$ mathematically as the process whose distribution is the limiting distribution of the previous Brownian particle. It has the following properties: for all open $A \subset R^3$

$$P\{\mathbf{x}(t) \in A \mid \mathbf{x}(0) = \mathbf{x}_0\} = (4\pi Dt)^{-3/2} \cdot \int_A e^{-|\mathbf{x}-\mathbf{x}_0|^2/(4Dt)}\, d\mathbf{x}. \tag{2.12}$$

The process $x(t)$ is a process of stationary independent increments and $x(t)-x(0)$ is a mean zero Gaussian process. Then

$$E \mid \mathbf{x}-\mathbf{x}_0 \mid^2 = Dt \tag{2.13}$$

and the paths of $\mathbf{x}(t)$ are continuous and the joint probability distribution of $(\mathbf{x}(t_1), \mathbf{x}(t_2), \cdots, \mathbf{x}(t_n))$ $(t_1 < t_2 < \cdots < t_n)$ is Gaussian. Let $w(t)$ be the one dimensional analogue of $\mathbf{x}(t)$ with $D = 1/2$ and $w(0) = 0$. The transition probability distribution of $w(t)$ is then given by

$$P\{a \leqq w(t) \leqq b \mid w(s) = x\} = [2\pi(t-s)]^{-1/2} \int_a^b e^{-(y-x)^2/(2(t-s))}\, dy.$$

The joint probability distribution of $(w(t_1), w(t_2), \cdots, w(t_n))$ is zero mean Gaussian so it is determined by the covariances $Ew(t_i)w(t_j)$. It is easy to determine the covariances using the independence of increments and the fact that $Ew^2(t) = t$ (cf. (2.13)). Indeed, assuming $t < s$ we have

$$\begin{aligned} Ew(t)w(s) &= E[w(s)-w(t)]w(t) + Ew^2(t) \\ &= E[w(s)-w(t)]Ew(t) + t = t = \min(t, s) \equiv t \wedge s. \end{aligned} \tag{2.14}$$

It can be easily seen that the following are Brownian motions

$$\begin{aligned} &\text{(i)}\ \ w_1(t) = w(t+s) - w(s), \\ &\text{(ii)}\ \ w_2(t) = cw(t/c^2), \qquad c = \text{const.} \end{aligned} \tag{2.15}$$

Further properties of $w(t)$ and the rigorous construction of a process $w(t)$ with the above properties are given in McKean [31]. It can be shown for example that

$$\limsup_{t\to\infty} w(t) = \infty, \qquad \liminf_{t\to\infty} w(t) = -\infty,$$

that $w(t)$ is nowhere differentiable etc. (cf. Itô and McKean [17]). We shall refer hence forward to $w(t)$ as the one dimensional Brownian motion, or Wiener process. Finally we remark that the solution $\mathbf{v}(t)$ of Langevin's equation is called the Ornstein–Uhlenbeck process. It leads to formula (2.9) which generalizes Einstein's result (2.11), which is valid for large t only, to all times. In particular, for short times

$$E|\mathbf{x}(t)-\mathbf{x}_0|^2 \approx \frac{3kT}{m}t^2.$$

This result is due to Ornstein and Fürth (cf. Ornstein and Uhlenbeck [36]).

3. The Itô calculus and its applications. The one dimensional Langevin equation is given by

$$\begin{aligned} \dot{y} &= -\beta y + q\dot{w} \\ y(0) &= y_0 \end{aligned} \tag{3.1}$$

where $q\dot{w}$ represents the "white noise" force due to collisions. Its solution is given by

$$y(t) = y_0\, e^{-\beta t} + q\int_0^t e^{-\beta(t-s)}\, dw(s). \tag{3.2}$$

The equation, as well as the solution do not represent well defined quantities since $w(t)$, though continuous, is nowhere differentiable. In the simple case of (3.2) this difficulty can be overcome by integration by parts, so that the form

$$y(t) = y_0\, e^{-\beta t} + qw(t) - \beta q\int_0^t w(s)\, e^{-\beta(t-s)}\, ds \tag{3.2'}$$

can be taken to be the solution of the integrated form of (3.1)

$$y(t) = y_0 - \beta\int_0^t y(s)\, ds + qw(t). \tag{3.1'}$$

This procedure becomes impossible if the integrand $e^{-\beta(t-s)}$ in (3.2) is replaced by a function of $w(t)$, or if q in (3.1) is a function of y or $w(t)$. To overcome this difficulty the following construction, due to Itô (cf. McKean [31]) is made. Let $f(t)$ be a random process such that $f(t)$ is independent of all the increments $w(t+s)-w(t)$, $s>0$ for each t. Then we say that $f(t)$ is *nonanticipating*. Let $H_2[0, T]$ be the class of all nonanticipating measurable functions $f(t)$ such that

$$\int_0^T Ef^2(t)\, dt < \infty.$$

Let $f(t)$ be a right continuous step function in $H_2[0, T]$, i.e. let

$$f(t) = \sum_{i=0}^{n-1} f_i \chi_{[t_i, t_{i+1})}(t),$$

where

$$\chi_{[t_i,t_{i+1})}(t) = 1 \quad \text{if } t_i \leqq t < t_{i+1}$$

and

$$\chi_{[t_i,\, t_{i+1})}(t) = 0 \quad \text{otherwise}, \qquad 0 = t_0 < t_1 < \cdots < t_n = T.$$

Then we set

$$\int_0^T f(t)\, dw(t) = \sum_{i=0}^{n-1} f_i[w(t_{i+1}) - w(t_i)]. \tag{3.3}$$

It follows that

$$E\int_0^T f(t)\, dw(t) = 0 \tag{3.4}$$

and

$$E\left[\int_0^T f(t)\, dw(t)\right]^2 = \sum_{i<j} Ef_i f_j\, \Delta_i w\, \Delta_j w,$$

where $\Delta_i w = w(t_{i+1}) - w(t_i)$. Since increments are independent and $f(t)$ is nonanticipating we have by property (i) and (2.4)

$$E\left[\int_0^T f(t)\, dw(t)\right]^2 = \sum_{i=0}^{n-1} Ef_i^2\, \Delta t_i = \int_0^T Ef^2(t)\, dt, \tag{3.5}$$

where $\Delta t_i = t_{i+1} - t_i$. It can be shown that for any function $f(t)$ in $H_2[0, T]$ there is a sequence $\{f_n\}$ of step functions in $H_2[0, T]$ such that

$$\int_0^T E[f(t) - f_n(t)]^2\, dt \to 0 \quad \text{as } n \to \infty$$

and such that the sequence

$$\left\{\int_0^t f_n(s)\, dw(s)\right\}$$

converges uniformly in $0 \leqq t \leqq T$ almost surely (cf. McKean [31]). We set

$$\int_0^t f(s)\, dw(s) = \lim_{n\to\infty} \int_0^t f_n(s)\, dw(s), \tag{3.6}$$

thus obtaining a meaningful definition of an integral. Properties (3.4) and (3.5) hold for any $f(t) \in H_2[0, T]$ and the integral (3.6) is an almost surely continuous martingale as a function of t. The integral can be extended to all measurable and nonanticipating functions $f(t)$ which satisfy

$$P\left\{\int_0^T f^2(s)\, ds < \infty\right\} = 1.$$

This is done by setting $f_n(t) = f(t)$ if $t < S_n$ and $f_n(t) = 0$ if $t \geqq S_n$, where

$$S_n = \inf\left\{t \,\middle|\, \int_0^t f^2(s)\, ds \geqq n\right\}.$$

Then $f_n \in H_2(0, T)$ and one defines

$$\int_0^T f(s)\, dw(s) = \lim_{n\to\infty} \int_0^T f_n(s)\, dw(s).$$

The stochastic differential equation

$$\dot{y}(t) = a(y(t), t) + b(y(t), t)\dot{w}(t)$$

can now be defined by

$$y(t) = y_0 + \int_0^t a(y(s), s)\, ds + \int_0^t b(y(s), s)\, dw(s)$$

where a and b are elements of $H_2(0, T]$.

The basic rules of the Itô calculus are described next. We say that a process $x(t)$ has the differential

$$dx(t) = a(t)\, dt + b(t)\, dw(t), \qquad a, b \in H_2[0, T] \tag{3.7}$$

if

$$x(t_2) - x(t_1) = \int_{t_1}^{t_2} a(s)\, ds + \int_{t_1}^{t_2} b(s)\, dw(s)$$

for all $0 \leqq t_1 \leqq t_2 \leqq T$. Let

$$x_i(t) = a_i(t)\, dt + b_i(t)\, dw(t), \qquad (i = 1, 2).$$

Then the product rule for differentials (cf. Gihman and Skorohod [13]) is given by

$$d[x_1(t)x_2(t)] = x_1(t)\, dx_2(t) + x_2(t)\, dx(t_1) + b_1(t)b_2(t)\, dt.$$

In particular

$$dw^2(t) = 2w(t)\, dw(t) + 1\, dt,$$

$$\int_{t_1}^{t_2} w(t)\, dw(t) = \frac{1}{2}[w^2(t_2) - w^2(t_1)] - \frac{1}{2}(t_2 - t_1),$$

unlike the classical calculus.

The chain rule, known as Itô's formula, is given by

$$\begin{aligned} df(x(t), t) = &\left[\frac{\partial f}{\partial t}(x(t), t) + a(t)\frac{\partial f}{\partial x}(x(t), t) + \frac{1}{2}b^2(t)\frac{\partial^2 f}{\partial x^2}(x(t), t)\right] dt \\ &+ b(t)\frac{\partial f}{\partial x}(x(t), t)\, dw(t), \end{aligned} \tag{3.8}$$

where $f(x, t)$ is a smooth function of x and t, and $x(t)$ has the differential (3.7). If $\mathbf{w}(t) = [w_1(t), w_2(t), \cdots, w_n(t)]^T$ is a vector of independent Brownian motions and the vector $\mathbf{x}(t) = [x_1(t), x_2(t), \cdots, x_n(t)]^T$ has the differential

$$d\mathbf{x}(t) = \mathbf{a}(t)\, dt + \mathbf{B}(t)\, d\mathbf{w}(t) \tag{3.7'}$$

where $\mathbf{a}(t) = [a_1(t), a_2(t), \cdots, a_n(t)]^T$ and $\mathbf{B}(t) = \{b_{ij}(t)\}_{i,j \leqq n}$ is a matrix, then Itô's formula is given by

$$df(\mathbf{x}(t), t) = Lf(\mathbf{x}, t)\, dt + \mathbf{M}f(\mathbf{x}, t)\, d\mathbf{w}(t), \tag{3.8'}$$

where

$$Lf=\frac{\partial f}{\partial t}+\sum_{i=1}^{n} a_i\frac{\partial f}{\partial x_i}+\sum_{i,j}\sigma_{ij}\frac{\partial^2 f}{\partial x_i\partial x_j}, \tag{3.9}$$

$$\sigma_{ij}=\frac{1}{2}\{BB^T\}_{ij}, \quad \text{and} \quad \mathbf{M}f\,d\mathbf{w}=\sum_{i,j} b_{ij}\frac{\partial f}{\partial x_i}\,dw_j. \tag{3.10}$$

The coefficients $\mathbf{a}$ and $\mathbf{B}$ may in general depend on $\mathbf{x}$, and indeed, very often they depend on $\mathbf{x}$ but not on t (the so called autonomic case). Two important consequences of Itô's formula are as follows. Let $\mathbf{x}(t)$ be a differentiable process in the sense of (3.7′) where $\mathbf{a}$ and $\mathbf{B}$ depend on $\mathbf{x}(t)$. Assume that $\mathbf{x}(0)\equiv\mathbf{x}\in\Omega$ where Ω is a bounded domain in R^n with smooth boundary $\partial\Omega$. Let $\tau_{\mathbf{x}}$ be the first time $\mathbf{x}(t)$ hits the boundary $\partial\Omega$, i.e. $\tau_{\mathbf{x}}=\inf\{t\mid \mathbf{x}(t)\in\partial\Omega,\ \mathbf{x}(0)=\mathbf{x}\}$. The expectation of $\tau_{\mathbf{x}}$ can be found by solving a backward parabolic or elliptic boundary value problem. For, let $v(\mathbf{x},t)$ be the solution of the problem

$$\begin{aligned} Lv(\mathbf{x},t)&=-1 \quad \text{in } \Omega\times(0,\infty)\equiv Q,\\ v(\mathbf{x},t)&=0 \quad \text{on } \partial\Omega\times(0,\infty). \end{aligned} \tag{3.11}$$

Then, using the integrated form of Itô's formula (3.11) with $f(\mathbf{x},t)=v(\mathbf{x},t)$ we obtain for all $t<\tau_{\mathbf{x}}$

$$v(\mathbf{x}(t),t)=v(\mathbf{x},0)+\int_0^t Lv\,ds+\int_0^L Mv\,dw(s);$$

hence, setting, as we may (cf. Gihman and Skorohod [13]) $t=\tau_{\mathbf{x}}$, taking expectation and using (3.4) we obtain

$$Ev(\mathbf{x}(\tau_{\mathbf{x}}),\tau_{\mathbf{x}})=v(\mathbf{x},0)+E\int_0^{\tau_{\mathbf{x}}}(-1)\,ds.$$

Since $\mathbf{x}(\tau_{\mathbf{x}})\in\partial\Omega$ we have $v(\mathbf{x}(\tau_{\mathbf{x}}),\tau_{\mathbf{x}})=0$

so

$$v(\mathbf{x},0)=E\tau_{\mathbf{x}}. \tag{3.12}$$

Formula (3.12) is due to Dynkin (cf. Dynkin [9]). If $\mathbf{a}$ and $\mathbf{B}$ are functions of $\mathbf{x}$, (3.11) becomes an elliptic boundary value problem. The existence of bounded solutions to (3.11) implies that the process $\mathbf{x}(t)$ hits the boundary $\partial\Omega$ in finite time almost surely. In case $\mathbf{a}$ and $\mathbf{B}$ depend on $\mathbf{x}$ and t, (3.11) is a backward parabolic boundary value problem, for which existence theory is discussed in Friedman and Schuss [12] and Schuss [41], [42]. Next, let $p(\mathbf{x},\mathbf{y})$ be the probability density of points $\mathbf{y}$ on $\partial\Omega$ where $\mathbf{x}(t)$ hits $\partial\Omega$ for the first time, given $\mathbf{x}(0)=\mathbf{x}$. More precisely, let $\Gamma\subset\partial\Omega$; then

$$P(\mathbf{x}(\tau_{\mathbf{x}})\in\Gamma\mid\mathbf{x}(0)=\mathbf{x})=\int_\Gamma p(\mathbf{x},\mathbf{y})\,dS_{\mathbf{y}}.$$

It follows that $p(\mathbf{x},\mathbf{y})$ is Green's function of the Dirichlet problem

$$\begin{aligned} Lu&=0 \quad \text{in } \Omega\\ u&=f(\mathbf{x}) \quad \text{on } \partial\Omega \end{aligned} \tag{3.13}$$

(assume for simplicity that $\mathbf{a}$ and $\mathbf{B}$ are independent of t). Indeed, let $u(\mathbf{x})$ be the solution

of (3.13) for some smooth function $f(\mathbf{x})$. Then, using Itô's formula as above we have

$$Eu(\mathbf{x}(\tau_{\mathbf{x}})) = u(\mathbf{x}) + E\int_0^{\tau_{\mathbf{x}}} Lu\, dt + E\int_0^{\tau_{\mathbf{x}}} \mathbf{M}u\, d\mathbf{w} = u(\mathbf{x}).$$

Now, since $\mathbf{x}(\tau_{\mathbf{x}}) \in \partial\Omega$ we have

$$u(\mathbf{x}) = Ef(\mathbf{x}(\tau_{\mathbf{x}})) = \int_{\partial\Omega} f(\mathbf{y}) P(\mathbf{x}(\tau_{\mathbf{x}}) \in dS_{\mathbf{y}} \mid \mathbf{x}(0) = \mathbf{x}) \tag{3.14}$$

where $dS_{\mathbf{y}}$ is a surface area element at $\mathbf{y}$ in $\partial\Omega$. Hence

$$u(\mathbf{x}) = \int_{\partial\Omega} f(\mathbf{y}) p(\mathbf{x}, \mathbf{y})\, dS_{\mathbf{y}},$$

which means that $p(\mathbf{x}, \mathbf{y})$ is Green's function for (3.13). The probability distribution of $\tau_{\mathbf{x}}$ can also be found by similar considerations. Namely, let $w(\mathbf{x}, t)$ be the solution of the backward parabolic problem

$$\begin{aligned} Lw(\mathbf{x}, t) &= 0 \qquad 0 \leqq t \leqq T, \quad x \in \Omega, \\ w(\mathbf{x}, t) &= 1 \qquad x \in \partial\Omega, \qquad 0 \leqq t < T, \\ w(\mathbf{x}, T) &= 0 \qquad x \in \Omega. \end{aligned} \tag{3.15}$$

Then, using Itô's formula we find that

$$Ew(\mathbf{x}(\tau_{\mathbf{x}} \wedge T), \tau_{\mathbf{x}} \wedge T) = w(\mathbf{x}, 0),$$

but

$$\begin{aligned} Ew(\mathbf{x}(\tau_{\mathbf{x}} \wedge T), \tau_{\mathbf{x}} \wedge T) &= w(\mathbf{x}, T) P(\tau_{\mathbf{x}} \wedge T = T) \\ &\quad + \int_{\partial\Omega}\int_0^T w(\mathbf{y}, z) P(\mathbf{x}(\tau_{\mathbf{x}}) \in dS_{\mathbf{y}}, \tau_{\mathbf{x}} \in dz) = P(\tau_{\mathbf{x}} < T). \end{aligned}$$

Thus

$$P(\tau_{\mathbf{x}} < t) = w(\mathbf{x}, 0).$$

4. Stochastic differential equations and partial differential equations. If $\mathbf{a}$ and $\mathbf{B}$ in (3.7′) are functions of $\mathbf{x}(t)$ and t then (3.7′) becomes a stochastic differential equation. More precisely, the integrated form of (3.7′) is the integral equation

$$\mathbf{x}(t) = \mathbf{x}(s) + \int_s^t \mathbf{a}(\mathbf{x}(z), z)\, dz + \int_s^t \mathbf{B}(\mathbf{x}(z), z)\, d\mathbf{w}(z) \tag{4.1}$$

which defines (3.7′) as a differential equation. Under certain smoothness and growth conditions on $\mathbf{a}$ and $\mathbf{B}$ there exists a unique solution to (4.1) (cf. Gihman and Skorohod [13]). It can be shown that the solution is a diffusion process with drift coefficient $\mathbf{a}(\mathbf{x}, t)$ and diffusion tensor $\boldsymbol{\sigma} = \frac{1}{2}(\mathbf{B}\mathbf{B}^T)(\mathbf{x}, t)$. The converse is also true; if $\mathbf{x}(t)$ is a diffusion process with sufficiently smooth coefficients $\mathbf{a}(\mathbf{x}, t)$ and $\boldsymbol{\sigma}(\mathbf{x}, t)$, $\boldsymbol{\sigma}$ is strictly positive definite and $\boldsymbol{\sigma}^{-1}$ is bounded then $\mathbf{x}(t)$ is the solution of (4.1) where $\mathbf{B}$ is a matrix such that $\boldsymbol{\sigma} = \frac{1}{2}\mathbf{B}\mathbf{B}^T$ [13]. To explain the nature of the information we look for in stochastic differential equations consider the simplest one dimensional case

$$dx(t) = a(t)\, dt + b(t)\, dw(t), \qquad x(0) = x_0$$

where $a(t)$ and $b(t)$ are deterministic functions. The solution is given explicitly by

$$x(t) = x_0 + \int_0^t a(s)\, ds + \int_0^t b(s)\, dw(s). \tag{4.2}$$

The stochastic integral in (4.5) is the limit of sums $\sum_i b(s_i)[w(s_{i+1})-w(s_i)]$ as described in § 3. This sum is a linear combination of zero mean independent Gaussian variables, so it is a Gaussian variable; hence the limit is a zero mean Gaussian variable. The variance of the stochastic integral is given by (3.5), so

$$Ex(t)=x_0+\int_0^t a(s)\,ds$$

by (3.4), and

$$\operatorname{Var} x(t)=E[x(t)-Ex(t)]^2=\int_0^t b(s)^2\,ds.$$

It can be shown that the solution $\mathbf{x}(t)$ of (4.1) has, under certain smoothness conditions, a *transition probability density* $(p\mathbf{x}, s, \mathbf{y}, t)$ such that

$$P(\mathbf{x}(t)\in A \mid \mathbf{x}(s)=\mathbf{x})=\int_A p(\mathbf{x}, s, \mathbf{y}, t)\,d\mathbf{y} \qquad (s<t).$$

In the given example $x(t)$ is Gaussian so that

$$p(x, s, y, t)=\left[2\pi\int_s^t b^2(z)\,dz\right]^{-1/2}\exp\left[-\left(y-x-\int_s^t a(z)\,dz\right)^2\Big/2\int_s^t b^2(z)\,dz\right].$$

Hence

$$\frac{\partial p}{\partial t}=\frac{1}{2}b^2(t)\frac{\partial^2 p}{\partial y^2}+a(t)\frac{\partial p}{\partial y},$$

$$p(x, s, y, t)\to\delta(x-y) \quad \text{as } t\downarrow s.$$

The basic information about the solution is not necessarily a formula for the solution, but rather its probability distribution, moments etc. Another example of a stochastic differential equation that can be solved explicitly is Langevin's equation for the Brownian harmonic oscillator

$$\ddot{x}+\beta\dot{x}+\omega^2 x=\sqrt{\frac{2\beta kT}{m}}\dot{w} \tag{4.3}$$

where β, T and m are the same as in § 2 and ω is the natural frequency of the oscillator. Equation (4.3) is equivalent to the Itô system of equations

$$dx=y\,dt,$$

$$dy=-(\beta y+\omega^2 x)\,dt+\sqrt{\frac{2\beta kT}{m}}\,dw.$$

In this case the vector $\mathbf{a}$ is given by $a_1=y$, $a_2=-\beta\mathbf{y}-\omega^2 x$, and the matrix $\mathbf{B}$ is given by

$$\mathbf{B}=\begin{pmatrix}0 & 0\\ 0 & q\end{pmatrix} \quad \text{where } q=\sqrt{\frac{2\beta kT}{m}}.$$

The solution is given by

$$x=\frac{-1}{\mu_1-\mu_2}[(x_0\mu_2-y_0)\,e^{\mu_1 t}-(x_0\mu_1-y_0)\,e^{\mu_2 t}]+\int_0^t \Psi(s)\,dw(s),$$

where

$$\mu_{1,2} = -\tfrac{1}{2}\beta \pm (\tfrac{1}{4}\beta^2 - \omega^2)^{1/2},$$

$$\Psi(s) = \frac{q}{\mu_1 - \mu_2}[e^{\mu_1(t-s)} - e^{\mu_2(t-s)}].$$

Thus

$$E_{x_0,y_0}x(t) \to 0, \qquad E_{x_0,y_0}y(t) \to 0$$

$$E_{x_0,y_0}x^2(t) \to \frac{kT}{m\omega^2}$$

$$E_{x_0,y_0}y^2(t) \to \frac{kT}{m} \quad \text{as } t \to \infty$$

(cf. Chandrasekhar [6]). Equation (4.3) can be used as a model for a motion of an atom performing thermal vibrations in a crystalline lattice. In this case β can no longer be considered a viscosity coefficient but rather it represents the rate of dissipation of the kinetic energy of an atom by interaction with the lattice through internuclear forces (cf. § 7). Several important applications of the above elementary theory of stochastic differential equations are presented in (Chandrasekhar [6]).

In the general case the transition probability density $p(\mathbf{x}, s, \mathbf{y}, t)$ satisfies the *Fokker–Planck* equation with respect to the "forward variables" $(\mathbf{y}, t)$

$$\partial p/\partial t = -\sum_i \partial[a_i(\mathbf{y}, t)p(\mathbf{x}, s, \mathbf{y}, t)]/\partial y_i + \sum_{i,j} \partial^2[\sigma_{ij}(\mathbf{y}, t)p(\mathbf{x}, s, \mathbf{y}, t)]/\partial y_i \partial y_j,$$

$$p(\mathbf{x}, s, \mathbf{y}, t) \to \delta(\mathbf{x} - \mathbf{y}) \quad \text{as } t \downarrow s. \tag{4.4}$$

Equation (4.4) is called also the *forward Kolmogorov* equation. The density $p(\mathbf{x}, s, \mathbf{y}, t)$ satisfies the *backward Kolmogorov* equation with respect to the "backward variables" $(\mathbf{x}, s)$

$$\partial p/\partial ds + \sum_i a_i(\mathbf{x}, s)\partial p/\partial x_i + \sum_{i,j} \sigma_{ij}(\mathbf{x}, s)\partial^2 p/\partial x_i \partial x_j = 0, \tag{4.5}$$

$$p(\mathbf{x}, s, \mathbf{y}, t) \to \delta(\mathbf{x} - \mathbf{y}) \quad \text{as } s \uparrow t. \tag{4.6}$$

If certain behavior at the boundary $\partial\Omega$ of a bounded domain Ω is imposed on $\mathbf{x}(t)$ then $p(\mathbf{x}, s, \mathbf{y}, t)$ satisfies some boundary conditions. Thus if $\partial\Omega$ is a perfectly absorbing boundary, i.e.

$$P(\mathbf{x}(t) \in A \mid \mathbf{x}(s) \in \partial\Omega) = 0$$

for any $A \subset \Omega$ and $t > s$ then $p(\mathbf{x}, s, \mathbf{y}, t) = 0$ for all $\mathbf{x} \in \partial\Omega$, $\mathbf{y} \in \Omega$ and $t > s$. If $\partial\Omega$ is an instantanously reflecting boundary then

$$\frac{\partial p}{\partial \boldsymbol{\gamma}_{\mathbf{x}}}(\mathbf{x}, s, \mathbf{y}, t) = 0 \qquad \mathbf{x} \in \partial\Omega, \quad \mathbf{y} \in \Omega, \quad t > s.$$

Here $\partial/\partial\gamma_{\mathbf{x}}$ is the normal derivative at $x \in \partial\Omega$ (cf. Gihman and Skorohod [13], Mandl [26], Anderson and Orey [1]). Formula (3.12) can be derived directly from (4.5) as

follows. Assume $\partial\Omega$ is an absorbing boundary, then, in the autonomic case,

$$E\tau_{\mathbf{x}} = \int_0^\infty t d_t P(\tau_{\mathbf{x}} < t) = \int_0^\infty P(\tau_{\mathbf{x}} \geqq t)\, dt = \int_0^\infty P(\mathbf{x}(s) \in \Omega,\ s < t \mid \mathbf{x}(0) = x)\, dt$$

$$= \int_0^\infty \int_\Omega p(\mathbf{x}, 0, \mathbf{y}, t)\, d\mathbf{y}\, dt.$$

Integrating (4.3) with respect to s and with respect to y over Q and using (4.6) we obtain (3.12) where $v(\mathbf{x}) = E\tau_{\mathbf{x}}$ satisfies (3.11). Equations (3.12) and (3.14) are representation formulas for solutions of partial differential equations by solutions of stochastic differential equations. For other representation formulas (cf. Gihman and Skorohod [13]).

5. The exit problem in mathematical physics. Following the attempts of Kramers [22] we construct a diffusion model for chemical reactions. A particle inside a molecule is held by chemical bonds and may be considered at rest or performing small oscillations about a stable equilibrium. In a chemical reaction external forces, such as the forces created in molecular collisions, may activate the particle to such a degree that it overcomes the chemical bonds and leaves the molecule. Once outside the molecule such a particle either forms a new bond and remains at a more stable equilibrium state or is removed permanently from the molecule by other means, such as an electrostatic field. The rate at which the external forces push such particles over the edge of the potential well in which they initially rest determines the kinetics of the reaction. If the particle has n degrees of freedom its motion can be described as that of a particle in the $2n$-dimensional phase space, that is by n independent displacement coordinates $\mathbf{x} = (x_1, \cdots, x_n)$ and by n velocity coordinates $\mathbf{y} = d\mathbf{x}/dt$. The potential well confining the particle may consist of a succession of holes and barriers through which the particle passes before it escapes. This is the case of successive chemical reactions. Here the reaction may be considered complete only after the highest potential barrier has been surmounted. The energy which the initial reactants must acquire before they can surmount the highest barrier separating them from the final products is called the *activation energy*. (See Figs. 5.1, 5.2 and 5.3.)

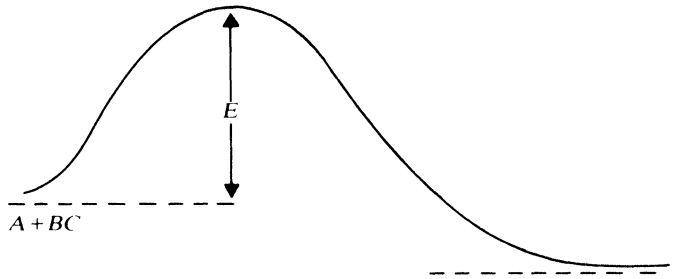

FIG. 5.1. *Potential barrier for a chemical reaction.*

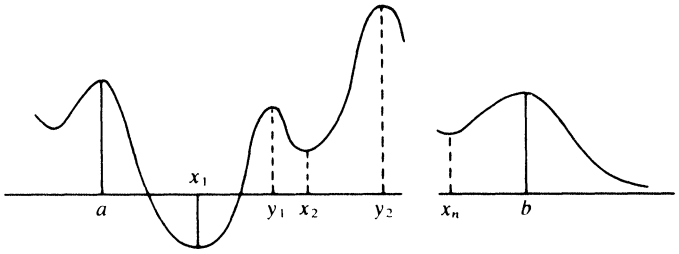

FIG. 5.2. *Potential for successive reactions.*

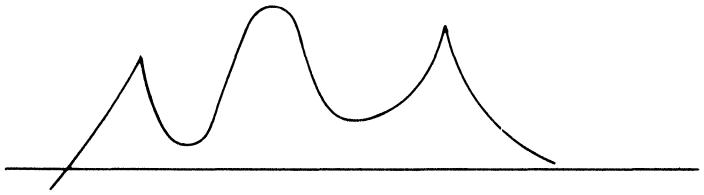

FIG. 5.3. *Potential barrier with sharp edges.*

The presence of intermediate states is inconsequential except in so far as such a state contains an appreciable fraction of the total molecules, which makes them really part of the initial state. For multiatomic molecules the potential energy is a function of the n independent internuclear distances measured from some arbitrary origin. In this case there are many directions of escape over the potential barrier in R^n. The different directions correspond to different chemical reactions. Such is the case where the same activation energy is required for the splitting of any of the three equivalent H atoms in CH_3F (cf. Benson [2], Glasstone [15]).

If the potential barrier is very sharp we may consider the forces to be discontinuous, so that once the bond is broken the force changes abruptly from attraction to repulsion. We shall compute for such models the rate of escape of particles over the barrier, thus giving the escape rate as a function of the potential well and of the temperature (i.e. as a function of the intensity of the collisions). In particular we shall find the effect of the stereometry of the potential well on the reaction rate and on the composition of the final products. We shall assume that the medium surrounding the molecule is in thermal equilibrium so that the velocity distribution of the particles is Maxwellian (in the n components $\mathbf{y}_n$). To be more specific we describe the motion of a chemically bound particle by the Langevin equation

$$\begin{aligned} \frac{d\mathbf{x}}{dt} &= \mathbf{y}, \\ \frac{d\mathbf{y}}{dt} &= -\beta\mathbf{y} - \nabla\Phi(\mathbf{x}) + \sqrt{\frac{2\beta kT}{m}}\,\dot{\mathbf{w}}. \end{aligned} \tag{5.1}$$

The function $\Phi(\mathbf{x})$ describes the chemical bonds and depends on the relative distances of atomic nuclei only. The expression $\sqrt{2\beta kT/m}\,\dot{\mathbf{w}}$ represents the white noise forces due to molecular collisions computed from Einstein's formula. In a typical case $\beta \sim 10^9 - 10^{10}$ while $kT/m \sim 10^1 - 10^3$ (cf. Chandrasekhar [6]). It follows that the Kramers–Smoluchowski approximation to Langevin's equation holds for large β. It is given by

$$\frac{d\mathbf{x}}{ds} = -\nabla\Phi(\mathbf{x}) + \sqrt{\frac{2kT}{m}}\,\dot{\mathbf{w}}(s) \tag{5.2}$$

where $t = \beta s$.

Several derivations of (5.2) exist in the mathematical literature: Chandrasekhar [6], Papanicolaou [37], Larsen and Schuss [23], et al.

The following derivation was communicated by the referee. Rescaling time by setting $t = \beta s$, noting that $(1/\sqrt{\beta})\mathbf{w}(\beta s) = \tilde{\mathbf{w}}(s) =$ Brownian motion (cf. § 2), and setting $\mathbf{y}^\beta(s) = \mathbf{y}(\beta s)$ and $\mathbf{x}^\beta(s) = \mathbf{x}(\beta s)$ in (7.1) we get

$$\begin{aligned} d\mathbf{x}^\beta(s) &= \beta\mathbf{y}^\beta(s)\,ds, \\ d\mathbf{y}^\beta(s) &= \beta p\,d\tilde{\mathbf{w}}(s) - \beta^2\mathbf{y}^\beta(s)\,ds - \beta\nabla\Phi(\mathbf{x}^\beta(s))\,ds, \end{aligned} \tag{5.3}$$

where $p^2 = 2kT/m$. Now let $\mathbf{z}^\beta(s)$ be the solution of

$$d\mathbf{z}^\beta(s) = \beta p\, d\tilde{\mathbf{w}}(s) - \beta^2 \mathbf{z}^\beta(s)\, ds, \qquad \mathbf{z}(0) = \mathbf{y}_0, \tag{5.4}$$

and set $\mathbf{y}^\beta(s) = \mathbf{z}^\beta(s) + \mathbf{v}^\beta(s)$. We will determine $\mathbf{v}^\beta(s)$:

$$\begin{aligned} d\mathbf{y}^\beta(s) &= d\mathbf{z}^\beta(s) + d\mathbf{v}^\beta(s) = \beta p\, d\tilde{\mathbf{w}}(s) - \beta^2 \mathbf{z}^\beta(s)\, ds + d\mathbf{v}^\beta(s) \\ &= \beta p\, d\tilde{\mathbf{w}}(s) - \beta^2 \mathbf{y}^\beta(s)\, ds + \beta^2 \mathbf{v}^\beta(s)\, ds + d\mathbf{v}^\beta(s). \end{aligned} \tag{5.5}$$

Substituting (5.5) in (5.3) we obtain an ordinary differential equation for $\mathbf{v}^\beta(s)$

$$d\mathbf{v}^\beta(s)/ds = -\beta^2 \mathbf{v}^\beta(s) - \beta \nabla \Phi(\mathbf{x}^\beta(s)).$$

The solution is given by

$$\mathbf{v}^\beta(s) = -\beta \int_0^s e^{-\beta^2(s-r)} \nabla \Phi(\mathbf{x}^\beta(r))\, dr.$$

The solution of (5.4) is given, as in (3.2), by

$$\mathbf{z}^\beta(s) = \mathbf{y}_0\, e^{-\beta^2 s} + p \int_0^s \beta\, e^{-\beta^2(s-r)}\, d\tilde{\mathbf{w}}(r).$$

Setting $\hat{\mathbf{y}}(s) = \beta \mathbf{y}^\beta(s)$ we obtain from (5.1)

$$\hat{\mathbf{y}}(s) = \frac{1}{\beta}\hat{\mathbf{y}}_0\, e^{-\beta^2 s} + p \int_0^s \beta^2\, e^{-\beta^2(s-r)}\, d\tilde{\mathbf{w}}(r) - \int_0^s \beta^2\, e^{-\beta^2(s-r)} \nabla \Phi(\mathbf{x}^\beta(r))\, dr.$$

Integrating $\hat{\mathbf{y}}(s)$ we obtain after some manipulations

$$\begin{aligned} \mathbf{x}^\beta(s) = \mathbf{x}_0 + \int_0^s \hat{\mathbf{y}}(s)\, ds &= \frac{1}{\beta^3}\hat{\mathbf{y}}_0(1 - e^{-\beta^2 s}) + p\beta^2 \int_0^s \tilde{\mathbf{w}}(r)\, e^{-\beta^2(s-r)}\, dr \\ &\quad - \int_0^s \int_0^t \beta^2\, e^{-\beta^2(t-r)} \nabla \Phi(\mathbf{x}^\beta(r))\, dr\, dt. \end{aligned}$$

Since $\beta^2\, e^{-\beta^2(s-r)} \to \delta(s-r)$ as $\beta \to \infty$, $s \geqq r$, we have $\mathbf{x}^\beta(s) \to \bar{\mathbf{x}}(s)$ where

$$\bar{\mathbf{x}}(s) = \bar{\mathbf{x}}_0 + p\tilde{\mathbf{w}}(s) - \int_0^s \nabla \Phi(\bar{\mathbf{x}}(r))\, dr,$$

which is equivalent to (5.2). The Fokker–Planck equation corresponding to (5.2) is given by

$$\frac{kT}{m}\Delta u + \nabla \cdot (\nabla \Phi u) = \partial u/\partial s.$$

It is called the Smoluchowski equation. It describes diffusion in a potential field (cf. Chandrasekhar [6]).

We shall assume that the depth of the potential well (the activation energy) is large relative to the quantity kT/m (here m is the reduced mass of the particle in a collision). More specifically, let Ω be the potential well, $\min_\Omega \Phi = 0$, $\max_{\partial\Omega} \Phi = Q$ where $\partial\Omega$ is the potential barrier. Then setting $-\nabla\Phi = -Q\nabla\phi \equiv Q\mathbf{b}$ we shall assume $kT/(mQ) \ll 1$. Hence, replacing s by $s' = Qs$ (thus $t \to \beta t/Q$) we obtain the equation

$$\frac{d\mathbf{x}}{dt} = \mathbf{b}(\mathbf{x}) + \varepsilon \frac{d\mathbf{w}}{dt} \tag{5.6}$$

where $\varepsilon = \sqrt{2kT/(mQ)}$ (we have used the Brownian scaling (2.15 ii) again).

On $\partial\Omega$ the force $\mathbf{b}(\mathbf{x})$ either vanishes or points in a direction parallel to $\partial\Omega$, but $\mathbf{b}(\mathbf{x})$ tends to repel particles away from the boundary on either side of $\partial\Omega$. If the potential has a cusp at $\partial\Omega$ then $\mathbf{b}$ does not vanish and $\mathbf{b}\cdot\boldsymbol{\gamma} < 0$ ($\boldsymbol{\gamma}$ = outer normal to $\partial\Omega$). In chemical terminology $\partial\Omega$ is called a *transition state*. The reaction rate constant k, first derived by Arrhenius, is the fraction of the particles entering the reaction per unit time. Thus in a first order reaction

$$k = -\left(\frac{1}{C}\right)\frac{dC}{dt}$$

where C is the concentration of the single reactant. Setting

$$\tau^\varepsilon = \inf\{t \mid \mathbf{x}^\varepsilon(t) \in \partial\Omega\}$$

where $\mathbf{x}^\varepsilon(t)$ is the solution of (5.6), $\mathbf{x}^\varepsilon(0) = \mathbf{x} \in \Omega$, we see that $1/\tau^\varepsilon_{\mathbf{x}}$ is the number of particles arriving at $\partial\Omega$ from $\mathbf{x}$ per unit time. Hence

$$k = \int_\Omega [\rho(\mathbf{x})/E_{\mathbf{x}}\tau^\varepsilon]\, d\mathbf{x}$$

where $\rho(\mathbf{x})$ is the relative concentration of particles in the well. Our purpose is to derive an asymptotic formula for k as $\varepsilon \to 0$. We may assume that initially all particles are concentrated at the bottom of the well $\mathbf{x} = \mathbf{0}$, so that

$$k = 1/E_0\tau^\varepsilon.$$

The function $v^\varepsilon(\mathbf{x}) = E_{\mathbf{x}}\tau^\varepsilon$ is the solution of the boundary value problem (3.11), so

$$\begin{aligned} L_\varepsilon v^\varepsilon = \varepsilon\, \Delta v^\varepsilon + b\cdot\nabla v^\varepsilon &= -1 \quad \text{in } \Omega \\ v &= 0 \quad \text{on } \partial\Omega. \end{aligned} \tag{5.7}$$

It can be shown (cf. Ludwig [25]) that $v^\varepsilon(0) = E_0\tau^\varepsilon \sim \lambda_\varepsilon^{-1}$ where λ_ε is the principal eigenvalue of L_ε. We shall use the method of Matkowsky and Schuss [29], [30] to compute $v^\varepsilon(\mathbf{x})$. Since $v^\varepsilon(\mathbf{x})$ grows exponentially as $\varepsilon \to 0$, we set $v^\varepsilon(x) = e^{-K/\varepsilon}W^\varepsilon(x)$ where $W^\varepsilon(\mathbf{x}) = C(\varepsilon)w^\varepsilon(\mathbf{x})$, $\max_\Omega w^\varepsilon = 1$, $C(\varepsilon) = o(e^{K/\varepsilon})$.

The function $w^\varepsilon(\mathbf{x})$ vanishes on the boundary $\partial\Omega$ but approaches 1 in Ω very rapidly as $\varepsilon \to 0$, so that $w^\varepsilon(\mathbf{x})$ is of boundary layer type. Using local coordinates near $\partial\Omega$ we find the boundary layer equation

$$\varepsilon w^\varepsilon_{yy} + yb_0 w^\varepsilon_y + L'w^\varepsilon = 0$$

where $y = -\text{dist}(\mathbf{x}, \Omega)$.

$$\mathbf{b}\cdot\boldsymbol{\gamma} = yb_0 + O(y^2), \qquad b_0 > 0.$$

The term $L'w^\varepsilon$ contains tangential derivatives and smaller terms in ε and is of boundary layer type. Rescaling $y = \sqrt{\varepsilon}z$ we obtain

$$\begin{aligned} w^\varepsilon_{zz} + zb_0 w^\varepsilon_z + L'w^\varepsilon &= 0, \\ w^\varepsilon(0) &= 0, \\ w(\infty) &= 1. \end{aligned}$$

Hence

$$w^\varepsilon(\mathbf{x}) = C_0(\varepsilon)\int_0^{y/\sqrt{\varepsilon}} e^{-s^2b_0/2}\, ds(1+o(1))\Big/\int_0^\infty e^{-y^2b_0/2}\, ds. \tag{5.8}$$

Since $\mathbf{b} = -\nabla\phi$ we can write equation (5.7) in the form

$$\varepsilon\nabla \cdot e^{-\phi/\varepsilon}\nabla v^{\varepsilon} = -e^{-\phi/\varepsilon}. \tag{5.7'}$$

Integrating over Ω and using the expansion (5.8) we obtain

$$-\int_{\Omega} e^{-\phi/\varepsilon}\,d\mathbf{x} = \varepsilon\int_{\partial\Omega} e^{-\phi/\varepsilon}\frac{\partial v^{\varepsilon}}{\partial\boldsymbol{\gamma}}\,dS = -e^{-K/\varepsilon}\sqrt{2\pi\varepsilon}C_0(\varepsilon)\int_{\partial\Omega} e^{-\phi/\varepsilon}b_0^{1/2}(\mathbf{x})\,dS_{\mathbf{x}}. \tag{5.7''}$$

Expanding asymptotically the Laplace type integrals we obtain (Olver [34])

$$(2\pi\varepsilon)^{n/2}\mathscr{H}^{-1/2}(\mathbf{0}) \sim (2\pi\varepsilon)^{n/2}\,e^{-K/\varepsilon}C_0(\varepsilon)\,e^{-\hat{\phi}/\varepsilon}\sum_i b_0^{1/2}(\mathbf{x}_i)H^{-1/2}(\mathbf{x}_i)$$

where $\hat{\phi} = \phi(\mathbf{x}_i) = \max_{\partial\Omega}\phi$,

$$\mathscr{H}(\mathbf{0}) = \det\frac{\partial^2\phi}{\partial x_i\partial_j} \qquad (i,j = 1,\cdots,n),$$

$$H(\mathbf{x}_k) = \det\frac{\partial^2\phi}{\partial x_i'\partial x_j'} \qquad (i,j = 1,\cdots,n-1),$$

and $\mathbf{x}' = (x_1',\cdots,x_{n-1}')$ are local coordinates in $\partial\Omega$. Thus $K = -\hat{\phi}$ and $C(\varepsilon) = \mathscr{H}(\mathbf{0})^{-1/2}/\sum_i b_0^{1/2}(\mathbf{x}_i)H^{-1/2}(\mathbf{x}_i)$; hence

$$E_0\tau^{\varepsilon} = \frac{\mathscr{H}^{-1/2}(\mathbf{0})}{\sum_i(\partial^2\phi/\partial\boldsymbol{\gamma}^2)^{1/2}H^{-1/2}(\mathbf{x}_i)}\,e^{\hat{\phi}/\varepsilon}. \tag{5.9}$$

The validity of the expansion (5.9) was proved rigorously by Kamin [20].

Since Φ is the potential per unit mass let $\Psi = m\Phi$ be the potential. Using the original time scale we obtain

$$k = \frac{Q}{\beta}\,(E_0\tau^{\varepsilon})^{-1} = \frac{1}{2\pi m\beta}\mathscr{H}^{1/2}(\mathbf{0})\sum_i\left(\frac{\partial^2\Psi}{\partial\boldsymbol{\gamma}^2}\right)^{1/2}H^{-1/2}(\mathbf{x}_i)\,e^{-\hat{\Psi}/kT}.$$

Here $\mathscr{H}$ and H are the Hessians of Ψ.

We see that the reaction rate is lower if viscosity is larger and if the particles are heavier. Note that the preexponential factor incorporates the geometry of the well, thus taking into account the fact that not all collisions are as likely to produce a reaction; this is the steric factor. Further formulas were derived by Matkowsky and Schuss [29], [30].

The probability distribution of exit points on $\partial\Omega$ will be discussed in the next problem of atomic migration in crystals. A crystal is a periodic structure of atoms arranged in a regular array, e.g. the cubic structure of sodium chloride (cf. Pauling [39]). We shall assume that a cell Ω can be identified in a crystal so that the structure is a repetitive pattern of identical cells. If an impurity atom is located in an interstitial position it moves through the crystal by squeezing its way past some of the host atoms surrounding it. This process is caused by the thermal vibrations of the structure (cf. Girifalco [14]).

Although the vibrational amplitude of a particular atom remains small most of the time, occasionally the atom acquires enough energy for its amplitude to become quite large. Such a fluctuation might arise when the atoms on one side of one atom sway simultaneously toward it and push it over the boundary of the cell into a neighboring one. Such an interstitial atom may be considered either resting or performing small

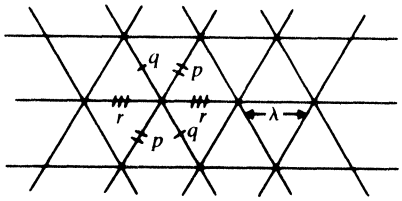

FIG. 5.4. *Nonisotropic lattice.*

oscillations at the bottom of the potential well of the interatomic forces. Each lattice atom may be considered a Brownian harmonic oscillator, so that the force acting on the interstitial atom may be considered to be of white noise type. It follows that (5.6) may be used to describe the motion of an impurity atom. Let $\bar{\tau}$ be the average time between a jump from one cell into another. Then the interstitial will perform a 3-dimensional random walk whose step size is the distance between the cells taken at time intervals $\bar{\tau}$ apart. In the case of vacancy migration one may consider a lattice with N sites as a single particle in the $3N$-dimensional space performing a random walk. If the cell structure is nonisotropic the jump frequencies will be different in different directions and the probability of passage through various saddle points separating the cells may be different. (See Fig. 5.4.) Let us assume that the lowest saddle points are located at points $\mathbf{z}_1, \cdots, \mathbf{z}_n$ on $\partial\Omega$ and the jump probability through $\mathbf{z}_i$ is p_i $(i = 1, 2, \cdots, n)$. We must have $n = 2m$, $\mathbf{z}_i = -z_{m+i}$, $p_i = p_{m+i}$, $i = 1, \cdots, m$. The probability of passage from a point $\mathbf{x}$ to a point $\mathbf{y}$ in the lattice in time $t + \Delta t = (n+1)\bar{\tau}$ satisfies the backward equation

$$p(\mathbf{x}, \mathbf{y}, t + \Delta t) = \sum_{i=1}^{n} p_i p(\mathbf{x} + z_i, \mathbf{y}, t).$$

Expanding in Taylor's series we obtain

$$\frac{\partial p}{\partial t} = \sum_{k=1}^{m} p_i \sum_{j,k} \frac{z_i^j z_i^k}{\bar{\tau}} \frac{\partial^2 p}{\partial x_j \partial x_k} + O\left(\frac{\lambda^2}{\bar{\tau}}\right)$$

where $\mathbf{z}_i = (z_i^1, z_i^2, z_i^3)^T$ and λ = diameter of a cell. We have therefore

$$\frac{\partial p}{\partial t} = \nabla \mathscr{D} \nabla p$$

where

$$\mathscr{D}_{jk} = \sum_{i=1}^{m} p_i z_i^j z_i^k / \bar{\tau}. \tag{5.10}$$

The matrix $\mathscr{D}$ is called the diffusion tensor. Since $\bar{\tau}$ is given by (5.9) we shall compute p_i now. The exit distribution is the Green's function for problem (3.13), which takes the form

$$\begin{aligned} \varepsilon\, \Delta u - \nabla \phi \cdot \nabla u &= 0 \quad \text{in } \Omega \\ u &= f \quad \text{on } \partial\Omega. \end{aligned} \tag{5.11}$$

We must have $\partial\phi/\partial\boldsymbol{\gamma} = 0$ on $\partial\Omega$

$$\phi = \phi(\mathbf{x}_0) - \tfrac{1}{2} y^2 b_0 + O(y^3), \qquad b_0 > 0,$$

in local coordinates near $\mathbf{x}_0 \in \partial\Omega$.

The reduced equation (5.11) is given by

$$-\nabla\phi \cdot \nabla u_0 = 0$$

or

$$\frac{du_0(\mathbf{x}(t))}{dt} = 0$$

where

$$\frac{d\mathbf{x}(t)}{dt} = -\nabla\phi. \tag{5.12}$$

Since all trajectories of (5.12) converge to the origin we must have

$$u_0 = \text{const.}$$

(cf. Matkowsky and Schuss [29], Kamin [1]). Consequently, a boundary layer is formed near $\partial\Omega$ as $\varepsilon \to 0$.

Writing (5.11) in local coordinates near $\partial\Omega$ we obtain

$$\varepsilon u_{yy} + yb_0 u_y + L'u = 0.$$

Rescaling $y = \eta\sqrt{\varepsilon}$ we find that

$$u_{\eta\eta} + \eta b_0 y_\eta + L'u = 0,$$
$$u(\mathbf{x}', 0) = f(\mathbf{x}')$$

where

$$(\mathbf{x}', 0) \in \partial\Omega,$$
$$u(x', \infty) = C = \text{const.}$$

Hence

$$u(\mathbf{x}', y) \sim C + (f(\mathbf{x}') - C) \int_{y/\sqrt{\varepsilon}}^{\infty} e^{-s^2 b_0/2}\, ds \Big/ \int_0^{\infty} e^{-s^2 b_0/2}\, ds (1 + o(1)). \tag{5.13}$$

Writing (5.11) in the form

$$\varepsilon \nabla \cdot e^{-\phi/\varepsilon} \nabla u = 0$$

and integrating over Ω we obtain

$$\int_{\partial\Omega} e^{-\phi/\varepsilon} \frac{\partial u}{\partial \boldsymbol{\gamma}}\, dS = 0. \tag{5.14}$$

Using (5.13) in (5.14) we obtain

$$\begin{aligned} C &= \lim_{\varepsilon \to 0} \int_{\partial\Omega} e^{-\phi/\varepsilon} f(\mathbf{x}) \left(\frac{\partial^2 \phi}{\partial \boldsymbol{\gamma}^2}\right)^{1/2} dS \Big/ \int_{\partial\Omega} e^{-\phi/\varepsilon} \left(\frac{\partial^2 \phi}{\partial \boldsymbol{\gamma}^2}\right)^{1/2} dS \\ &= \sum_i f(\mathbf{x}_i) \left(\frac{\partial^2 \phi(x_i)}{\partial \boldsymbol{\gamma}^2}\right)^{1/2} H^{-1/2}(\mathbf{x}_i) \Big/ \sum_i \left(\frac{\partial^2 \phi(\mathbf{x}_i)}{\partial \boldsymbol{\gamma}^2}\right)^{1/2} H^{-1/2}(x_i) \end{aligned} \tag{5.15}$$

where $\mathbf{x}_i$ are the saddle points in $\partial\Omega$ where $\phi = \min_{\partial\Omega} \phi$. This result is due to (Schuss and Matkowsky [30]).

It follows that

$$p(\tau_{\mathbf{x}}=\mathbf{y})=\sum_i\left(\frac{\partial^2\phi}{\partial\boldsymbol{\gamma}^2}(\mathbf{x}_i)\right)^{1/2}H^{-1/2}(\mathbf{x}_i)\delta(\mathbf{y}-\mathbf{x}_i)\Big/\int\sum\left(\frac{\partial^2\phi}{\partial\boldsymbol{\gamma}^2}(\mathbf{x}_i)\right)^{1/2}H^{-1/2}(\mathbf{x}_i)$$

or

$$p_i=\left(\frac{\partial^2\phi}{\partial\boldsymbol{\gamma}^2}(\mathbf{x}_i)\right)^{1/2}H^{-1/2}(\mathbf{x}_i)\Big/\sum_j\frac{\partial^2\phi}{\partial\boldsymbol{\gamma}^2}(\mathbf{x}_j)H^{-1/2}(\mathbf{x}_j). \tag{5.16}$$

It is obvious (cf. Kramers [22]) that if a single saddle point $\mathbf{x}_0$ exists on $\partial\Omega$ the particle is certain to escape at x_0. This was rigorously proved by Ventzel and Freidlin [47]. Combining (5.9), (5.10) and (5.16) we obtain

$$\mathscr{D}_{jk}=\frac{1}{2\pi m\beta}\mathscr{H}^{1/2}(\mathbf{0})\sum_i\left[\frac{\partial^2\phi}{\partial\boldsymbol{\gamma}^2}\right]^{1/2}H^{-1/2}(\mathbf{x}_i)x_i^jx_i^k\,e^{-\hat{\Psi}/(kT)}.$$

We see that $\mathscr{D}_{ij}$ is proportional to the product of the frequencies of oscillation at the bottom of the well ($\mathbf{x}=\mathbf{0}$), as $\mathscr{H}(\mathbf{0})$ is the product of the eigenvalues of the matrix $\partial^2\Psi/\partial x_i\partial x_j$ at $\mathbf{x}=\mathbf{0}$. The diffusion rate is inversely proportional to the product of the frequencies of oscillation at the saddle points $\mathbf{x}_i$ on $\partial\Omega$, but proportional to the imaginary frequency of oscillation in the direction across $\partial\Omega$, at a saddle point; the diffusion rate is slower if the particle is heavier. Here β is the slowing rate of the impurity particle due to its interaction with the lattice atoms. The same result was derived by Larsen and Schuss [23] directly from the Fokker–Planck equation. Similar results were obtained by Vineyard [48] and Glyde [16].

A chemical reaction or the motion of a vacancy (or the entire lattice) consists usually of a succession of jumps over intermediate barriers before a stable equilibrium is achieved. We shall show next how to compute the exit probabilities in such a case. Consider for simplicity the one dimensional case first. Equation (4.11) then takes the form

$$\begin{aligned}&\varepsilon u_\varepsilon''-\phi'u_\varepsilon'=0,\\ &u(a)=\alpha,\qquad u(b)=\beta\end{aligned} \tag{5.17}$$

where $\Omega=[a,b]$. Let ϕ have minima at $x_i, i=1,\cdots,n$ and maxima at $y_i, i=1,\cdots,n-1$. It is clear that $u_\varepsilon(x)\to C_i=\text{const.}$ as $\varepsilon\to 0, x_i<x<y_i$. We may expect therefore discontinuities to appear at x_i and y_i. Assume $-\phi'=A(x-z_i)^{k_i}+\cdots$ is Taylor's expansion of $-\phi'$ near $z_i=x_i$ of $z_i=y_i$. Rescaling the variable by setting $\xi=(x-z_i)/\varepsilon^\delta$ in (5.17) we obtain

$$\varepsilon^{1-2\delta}u_{\xi\xi}+[A_i\varepsilon^{\delta(k_i-1)}\xi^{k_i}+\cdots]u_\xi=0. \tag{5.18}$$

Hence, choosing $\delta=1/(k_i+1)$, we see that the dominant term in (5.18) satisfies the equation

$$u_{\xi\xi}+A_i\xi^{k_i}u_\xi=0 \tag{5.19}$$

near $\xi=0$. Equation (5.19) is the *internal layer equation* near z_i. Since

$$u_\xi\to C_i\quad\text{if } x_i<x<x_{i+1}$$

we must have

$$\begin{aligned}&u(\xi)\to C_{i-1}\quad\text{as } \xi\to-\infty\\ &u(\xi)\to C_i\ \xi\to\infty.\end{aligned}$$

The last two conditions match the *outer solutions* C_i, C_{i-1} by the internal layer $u(\xi)$. Since

$$u(\xi) = c_1 \int_0^{\xi} \exp\left[-A_i \xi^{k_i+1}/(k_i+1)\right] d\xi + c_2$$

we see that $c_1 = 0$ unless A_i is positive, i.e. unless ϕ has a minimum at z_i. Thus no discontinuities appear at y_i. At $x = x_i$ we have

$$c_1 = (C_i - C_{i-1})B_i \text{ and } c_2 = (C_i + C_{i-1})/2$$

where

$$B_i = \frac{1}{2} \Big/ \int_0^{\infty} \exp\left[-A_i \xi^{k_i+1}/(k_i+1)\right] d\xi$$

$$= A_i^{1/(k_i+1)} (k_i+1)^{k_i/(k_i+1)} \Big/ 2\Gamma\left(\frac{1}{k_i+1}\right).$$

Therefore the leading term in the expansion of u_ε near x_i is given by

$$u_\varepsilon(x) \sim (C_i + C_{i-1})/2 + (C_i - C_{i-1})B_i \cdot \int_0^{\xi} \exp\left[-A_i s^{k_i+1}/(k_i+1)\right] ds, \tag{5.20}$$

$$\xi = (x - x_i)\varepsilon^{-1/(k_i+1)}.$$

To determine C_i we multiply (5.17) by $e^{-\phi/\varepsilon}$ and integrate over (x_i, x_j) to obtain

$$e^{-\phi(x_i)/\varepsilon} u_\varepsilon'(x_i) - e^{-\phi(x_j)/\varepsilon} u_\varepsilon'(x_j) = 0,$$

and hence, using (5.20)

$$e^{-\phi(x_i)/\varepsilon} B_i (C_i - C_{i-1}) \varepsilon^{-1(k_i+1)} - e^{-\phi(x_j)/\varepsilon} B_j (C_j - C_{j-1}) \varepsilon^{-1/(k_j+1)} \sim 0.$$

If $\phi(x_i) = \min_{[a,b]} \phi$ then $C_i = C_{i-1}$ and no discontinuity appears at x_i. Assuming that $\phi(x_i) = \min_{[a,b]} \phi(x)$, $(i = 1, \cdots, n)$ we see that $C_i = C_{i-1}$ if $k_i = \max_j k_j$. Assuming $k_i = \max_j k_j$ we obtain the system

$$B_i(C_i - C_{i-1}) - B_j(C_j - C_{j-1}) = 0.$$

At $x = a$ we have

$$B_i(C_i - \alpha) - B_j(C_j - C_{j-1}) = 0$$

and a similar equation near $x = b$. In matrix notation we get

$$\begin{pmatrix} B_1 + B_2 & -B_2 & 0 & & \\ -B_2 & B_2 + B_3 & -B_3 0 & & \\ 0 & -B_3 & B_3 + B_4 & -B_4 0 & \\ & & \ddots & \ddots & \\ & & & -B_{n-2} B_{n-1} + B_n \end{pmatrix} \begin{pmatrix} C_1 \\ \cdot \\ \cdot \\ \cdot \\ C_{n-1} \end{pmatrix} = \begin{pmatrix} B_1 \alpha \\ 0 \\ \cdot \\ \cdot \\ 0 \\ B_n \beta \end{pmatrix}.$$

The solution is given by

$$C_j = (\alpha P_{n,j} + \beta Q_{n,j})/P_n$$

where

$$P_n = \sum_{j=1}^{n} \prod_{i=1}^{n} B_i \Big/ B_{n-j+1} \equiv \sum_{j=1}^{n} p_j,$$

$$P_{n,j} = \sum_{i=1}^{j} P_i, \qquad Q_{n,j} = P_n - P_{n,j}.$$

The exit probabilities are given by

$$P\{x_\varepsilon(\tau) = a \mid x_\varepsilon(0) = x\} = \sum_{j=0}^{n} D_j \chi_{(x_j, x_{j+1})}(x)$$

where $D_j = P_{n,j}/P_n$.

Remark. The problem of "resonance" in the boundary value problem

$$\varepsilon u'' - \phi' u' + gu = 0,$$
$$u(a) = \alpha, \qquad u(b) = \beta$$

or

$$\varepsilon\, \Delta u - \nabla\phi \cdot \nabla u + gu = 0 \quad \text{in } \Omega,$$
$$u = g \quad \text{on } \partial\Omega$$

can be treated by similar methods (cf. O'Malley [35], Matkowsky [28], Olver [33], Pridor and Schuss [40]).

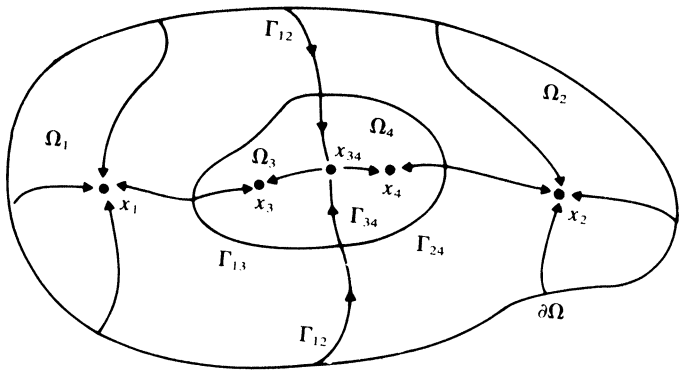

FIG. 5.5. *Potential well with multiple transition states.*

The case of multiple transition states in higher dimensions is treated along similar lines. (See Fig. 5.5.) The domain Ω is partitioned into domains of attraction Ω of the stable equilibrium points. We have $u_\varepsilon \to C_i$ in Ω_i and internal layers appear on the boundaries

$$\Gamma_{ij} = \partial\Omega_i \cap \partial\Omega_j$$

Using local coordinates near Γ_{ij} and rescaling the normal component

$$\xi = \omega\sqrt{\varepsilon}.$$

we obtain the internal layer equation

$$u_{\omega\omega} + \omega B(\eta) u_\omega + C(\eta) u_\eta = 0 \tag{5.21}$$

for (5.11). We have assumed that $\Omega \subset R^2$, and η is a tangential variable in Γ_{ij}, $B(\eta) > 0$. The change of variables

$$\mu = \exp \int_{\eta_0}^{\eta} \frac{ds}{C(s)}$$

reduces (5.21) to

$$u_{\omega\omega} + \omega\beta(\mu)u_\omega + \mu u_\mu = 0. \tag{5.22}$$

It can be shown that u is independent of the choice of η_0 (cf. Friedman and Schuss [12], Schuss [41], [42]). The matching conditions are

$$u(\omega, \mu) \to C_j \quad \text{as } \omega \to \infty,$$
$$u(\omega, \mu) \to C_i \quad \text{as } \omega \to -\infty.$$

Thus

$$u(\omega, \mu) = \frac{C_j - C_i}{2} u_1(\omega, \mu) + \frac{C_j + C_i}{2}$$

where $u_1(\omega, \mu)$ satisfies (5.22) and $u(\pm, \infty, \mu) = \pm 1$. The solution is given by

$$u_1(\omega, \mu) = \frac{1}{\sqrt{2\pi}} \int_0^{\omega\gamma(\mu)} e^{-s^2/2}\, ds$$

where $\gamma(\mu)$ is the solution of Bernoulli's equation

$$\gamma' + \frac{\beta(\mu)}{\mu}\gamma - \frac{1}{\mu}\gamma^3 = 0$$
$$\gamma(0) = \beta(0).$$

Multiplying (5.11) by $e^{-\phi/\varepsilon}$ and integrating over Ω, we obtain the system

$$\int_{\partial\Omega \cap \partial\Omega_i} e^{-\phi/\varepsilon} \left(\frac{\partial^2 \phi}{\partial \gamma^2}\right)^{1/2} (f - C_i)\, ds + \sum_j \frac{C_j - C_i}{2} \int_{\Gamma_{ij}} e^{-\phi/\varepsilon} \gamma(\mu(s))\, ds \sim 0.$$

This is a system of linear equations for C_j whose solution is given by

$$C_i = \int_{\partial\Omega} f\, dm_i(s)$$

where $m_i(s)$ is a measure on $\partial\Omega$. The form of m_i depends on quotients of integrals over $\partial\Omega$ and Γ_{ij} (cf. Matkowsky and Schuss [29], [30] for details, also Mangel and Ludwig [27]).

6. The phenomenon of cycle slipping in nonlinear filtering theory. The problem of nonlinear filtering of random signals from noisy measurements arises in many areas of engineering, such as radar, sonar, communications and optimal control.

In communication theory the signal, e.g. speech or music, is often modeled as a random process $x(t)$. More precisely, the voltage entering the modulator is a random process $x(t)$ and we denote by $P(x(t_1) < b_1, \cdots, x(t_n) < b_n)$ the probability that the voltage entering the modulator at times $t_1 < t_2 < \cdots < t_n$ satisfies the inequalities $x_i(t_i, \cdot) < b_i$; $(i = 1, 2, \cdots, n)$. It is a common practice to assume that $x(t)$ is a stationary

Gaussian process. Furthermore, $x(t)$ is often assumed to have a power spectrum function $S_x(\omega)$ given by

$$S_x(\omega) = \begin{cases} C & \text{if } |\omega| < k, \\ 0 & \text{otherwise,} \end{cases}$$

where C, and k are constants. Here

$$S_x(\omega) = \int_{-\infty}^{\infty} e^{-i\omega t} E[x(t)x(0)]\, dt$$

is the two sided spectral density. Since a realization of such a process $x(t)$ as a solution of an Itô differential equation is unknown we shall proceed as follows. Following Van Trees [46] we consider the Butterworth family of spectra

$$S_n(\omega) = 2n \sin(\pi/2n) \Big/ \left\{ k\left[\left(\frac{\omega}{k}\right)^{2n} + 1 \right] \right\}.$$

Obviously $S_n(\omega) \to S_x(\omega)$ as $n \to \infty$. It can be easily shown that for each n the stationary solution $x_n(t)$ of the equation

$$L_n x_n(t) = \dot{w}(t), \tag{6.1}$$

where L_n is an nth order linear differential operator with constant coefficients and $w(t)$ is a standard Brownian motion, has the spectral density $S_n(\omega)$. Equation (6.1) is equivalent to the system of stochastic Itô differential equations given by

$$d\mathbf{x}_n(t) = \mathbf{A}_n \mathbf{x}_n(t)\, dt + \mathbf{B}\, dw(t) \tag{6.2}$$

where

$$\mathbf{x}_n(t) = [x_n(t), \dot{x}_n(t), \cdots, x_n^{(n-1)}(t)]^T,$$

$\mathbf{B}$ is a constant vector and $\mathbf{A}$ is a constant matrix. We shall consider the case $n = 1$. In this case (6.2) reduces to (6.1), namely

$$dx(t) = -kx(t)\, dt + \sqrt{2k}\, dw_1(t),$$

$$x(0) = x_0$$

where $w_1(t)$ is the standard Wiener process. The initial condition x_0 is a zero mean Gaussian variable, $Ex_0^2 = 1$. The constant k expresses the bandwidth of the message $x(t)$.

We consider a problem arising in the theory of FM transmission, by describing the transmitted signal first. The FM transmitter integrates the signal $x(t)$ and adds a high frequency carrier to it, so the frequency modulated (FM) signal leaving the transmitter has the form

$$g = \sqrt{2} \sin\left(\omega_0 t + d_f \int_0^t x(s)\, ds\right) \equiv \sqrt{2} \sin[\omega_0 t + d_f \theta(t)].$$

Here ω_0 is the high frequency of the carrier, d_f is the frequency deviation, and we refer to the parameter $\beta = d_f/k$ as the modulation index. The FM demodulator we consider is based on the so called *phase-locked loop* (PLL), which was extensively studied by Viterbi [49] and Lindsey [24]. The PLL under consideration was proposed by Snyder [44]; its design is based on Kalman filtering considerations and has noise intensity dependent gains (cf. Fig. 6.3).

To clarify the action of the PLL and the derivation of the equations describing it we consider first a simpler version of the PLL (cf. Fig. 6.1).

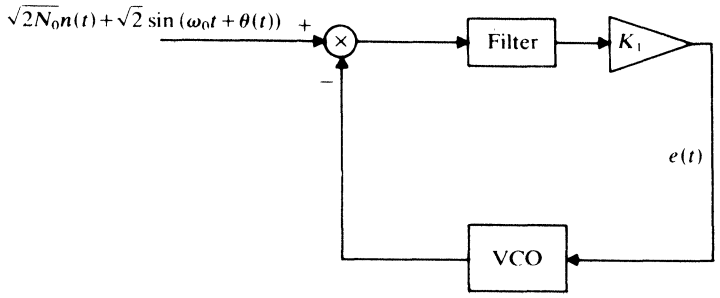

FIG. 6.1. *The PLL.*

The FM signal $g+\sqrt{2N_0}\,n(t)$ entering the loop contains additional white noise $\sqrt{2N_0}\,n(t)$, e.g. atmospheric disturbances, internal noise in the transmitter etc. Therefore, the noisy measurements process $y(t)$ is modeled by another Itô equation

$$dy(t)=g(x(t),t)\,dt+\sqrt{2N_0}\,dw_2(t)$$

where N_0 measures the noise intensity and $w_2(t)$ is another standard Wiener process, independent of $w_1(t)$. Thus the filtering problem is to estimate $x(t)$, given the noisy measurements $y(s)$, $0\leqq s\leqq t$.

It is well known (Viterbi [49]) that $n(t)$ can be represented by

$$n(t)=\sqrt{2}\,(n_1(t)\sin\omega_0 t+n_2(t)\cos\omega_0 t)$$

where $n_1(t)$ and $n_2(t)$ are independent white noise processes. The parameter N_0 measures the noise intensity. The term $1/N_0$ is called the signal to noise ratio (SNR). The output of the voltage controlled oscillator (VCO) is a cosine wave whose frequency is controlled by the input voltage $e(t)$, i.e.

$$H(t)=\sqrt{2}\,K_3\cos[\omega_0 t+\theta_2(t)]$$

where $\dot\theta_2(t)=K_2e(t)$. The constants K_i $(i=1,2,3)$ represent gains. The device $\otimes$ represents multiplication of the received signal $g+\sqrt{2N_0}\,n(t)$ by $H(t)$ with the result

$$\begin{aligned}[g+\sqrt{2N_0}\,n(t)]H(t)=2K_3\{&\sin[\theta_1(t)-\theta_2(t)]\\&-\sqrt{2N_0}\,n_1(t)\sin\theta_2(t)+\sqrt{2N_0}\,n_2(t)\cos\theta_2(t)\\&+\sin[2\omega_0 t+\theta_1(t)+\theta_2(t)]+\sqrt{2N_0}\,n_1(t)\sin[2\omega_0 t+\theta_2(t)]\\&+\sqrt{2N_0}\,n_2(t)\cos[2\omega_0 t+\theta_2(t)]\}.\end{aligned}$$

The low pass filter F supresses the high frequency terms so the filtered and amplified signal is given by

$$\begin{aligned}e(t)&=K_1K_3F(s)\{\sin[\theta_1(t)-\theta_2(t)]\\&\qquad-\sqrt{2N_0}\,n_1(t)\sin\theta_2(t)+\sqrt{2N_0}\,n_2(t)\cos\theta_2(t)\}\\&\equiv K_1K_3F(s)\sin\phi+\sqrt{2N_0}\,n'(t),\end{aligned}$$

where $F(s)$ is a linear operator (cf. Mikusinski [32]) which represents the effect of the

linear filter F (cf. Fig. 6.2). The term

$$n'(t) = -n_1(t)\sin\theta_2(t) + n_2(t)\cos\theta_2(t)$$

is also a white noise (Viterbi [49]), and $\phi = \theta_1 - \theta_2$ is the phase error. The block diagram model of the FM signal and the PLL is given by Fig. 6.2.

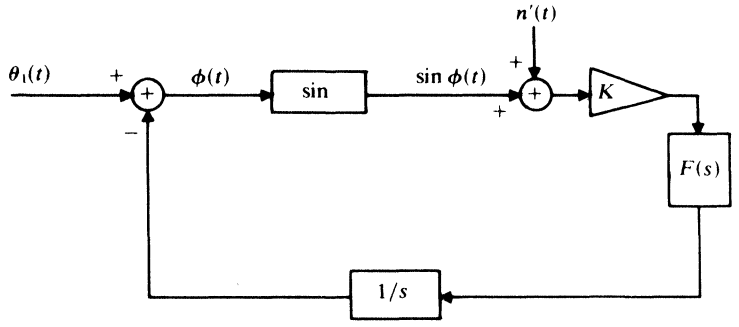

FIG. 6.2. *The Block diagram of the PLL.*

Here $K = K_1K_2K_3$. The filter $F(s)$ can be chosen in various ways; choosing $F(s)$ accordingly by Kalman filtering considerations (Snyder [44], Van Trees [46]) we obtain the PLL whose block diagram is given in Fig. 6.3.

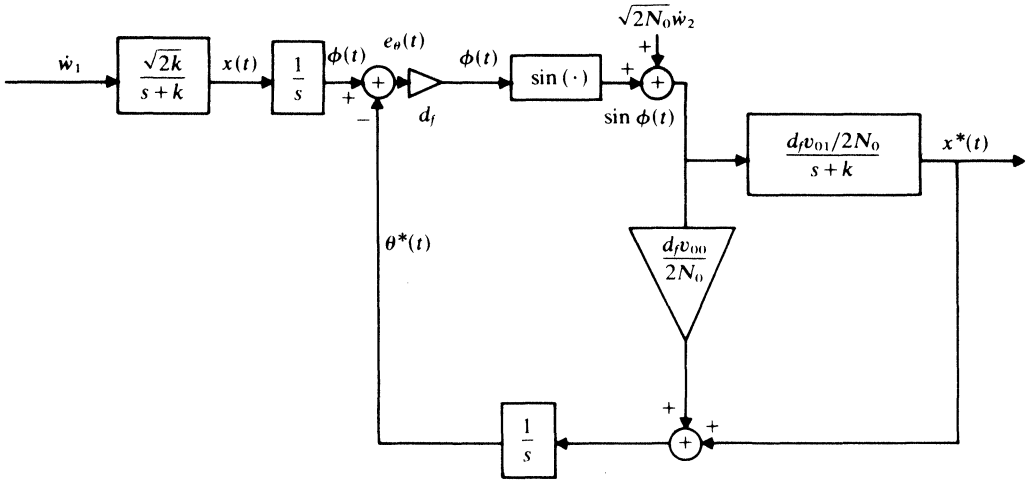

FIG. 6.3. *Block diagram of the suboptimal PLL.*

In the PLL of Fig. 6.3 we use the process $\theta^*(t)$ as an estimate of the phase $\theta(t) = \int_0^t x(s)\,ds$, and $x^*(t)$ as the estimate of the frequency $x(t)$. The parameter $\Lambda = 1/kN_0$ is referred to as the signal to noise ratio in the message bandwidth, and the loop gains v_{00} and v_{01} are given by

$$d_f^2 v_{00} = \frac{4\beta\Lambda^{-1/2}}{1+\sqrt{1+2\beta\Lambda^{1/2}}} \simeq 2\sqrt{2\beta}\Lambda^{-1/4}, \tag{6.3}$$

$$d_f v_{01} = 4\beta/(1+\sqrt{1+2\beta\Lambda^{1/2}})^2 \simeq 2\Lambda^{-1/2} \tag{6.4}$$

since in most practical cases $\beta\Lambda^{1/2} \gg 1$. To investigate the performance of the PLL we analyze the estimation error in frequency $e_x = x(t) - x^*(t)$ and the total phase error

$$\phi(t) = d_f(\theta(t) - \theta^*(t)).$$

The phases $\theta_1(t)$ and $\theta_2(t)$ of the PLL in Fig. 6.2 correspond to $d_f\theta(t)$ and $d_f\theta^*(t)$ respectively in the PLL of Fig. 6.3.

The system of equations describing the errors $e_x(t)$ and $\phi(t)$ is given by Snyder [44]

$$\begin{aligned} de_x = &-\left[ke_x + \frac{v_{01}d_f}{2N_0}\sin\phi\right]dt \\ &+\left[\sqrt{2k}\,dw_1 - \frac{v_{01}d_f}{2N_0}dw_2\right], \end{aligned} \tag{6.5}$$

$$d\phi = \left[d_f e_x - \frac{v_{00}d_f^2}{2N_0}\sin\phi\right]dt - \frac{v_{00}d^2f}{\sqrt{2N_0}}dw_2. \tag{6.6}$$

Using (6.3), (6.4), setting

$$\varepsilon = 2\sqrt{2\beta}\Lambda^{-3/4}, \qquad \xi = \sqrt{2\beta}\,e_x\Lambda^{-1/4}$$

and scaling the time by

$$t' = t/\gamma, \qquad \gamma = 1/(\sqrt{2\beta}\,k\Lambda^{1/4})$$

we get from (6.5) and (6.6) (cf. Bobrovsky and Schuss [3])

$$d\xi(t') = -(\delta\xi + \sin\phi)\,dt' + (dw_1' - dw_2')\sqrt{\varepsilon} \tag{6.7}$$

$$d\phi(t') = (\tfrac{1}{2}\xi - \sin\phi)\,dt' - dw_2'\sqrt{\varepsilon} \tag{6.8}$$

where $\delta = (\varepsilon/(8\beta^2))^{1/3}$, and $dw_i'(t') = (1/\sqrt{\gamma})\,dw_i(t)$ $(i = 1, 2)$, according to the Brownian scaling law (2.15) (ii). The drift vector in this case has the components b_1 and b_2, given by (6.9) and (6.10) respectively and the diffusion matrix σ_{ij} is given by $\sigma_{11} = 1$, $\sigma_{12} = \frac{1}{2}$ and $\sigma_{22} = \frac{1}{2}$ (cf. (3.9)).

The coefficients in (6.7) and (6.8) are periodic in ϕ, therefore a "skipping" of 2π in ϕ will leave the system unchanged. Since the frequency $x(t)$ is proportional to $\dot\theta$ an error of 2π in the estimate θ^* of θ will cause a sharp change in x^* which is heard as a "click". A natural measure of click frequency is the mean time $E\tau$ between clicks, whose computation is the object of this section. From the mathematical point of view the system (6.7), (6.8) represents a small stochastic perturbation of the dynamical system

$$\dot\xi = -\sin\phi - \delta\xi = b_1(\xi, \phi), \tag{6.9}$$

$$\dot\phi = \tfrac{1}{2}\xi - \sin\phi = b_2(\xi, \phi) \tag{6.10}$$

which has stable equilibria at $\xi = 0$, $\phi = 2\pi n$ $(n = 0, \pm 1, \cdots)$. All solutions of (6.9) and (6.10) which remain bounded as $t \to \infty$ converge to equilibrium points so that any trajectory which begins in the domain of attraction of a given stable equilibrium point will not cross into the domain of another one. However even the slightest stochastic perturbation is sure to cause such a crossing in finite time. The phenomenon of slipping cycles by the PLL can be described mathematically as an instability caused by stochastic forcing of a stable system. More precisely, the solution $(\xi(t), \phi(t))$ spends long time intervals near an attractive point, $\xi = 0$, $\phi = 0$, say, and we shall say therefore that a cycle slipping has occurred whenever a trajectory crosses into the domain of attraction

of $\xi = 0$, $\phi = \pm 2\pi$, say. If D is the domain of attraction of $\xi = 0$, $\phi = 0$ then the slip time is defined by

$$\tau = \inf\{t \mid (\xi(t), \phi(t)) \in \partial D\}$$

where ∂D is the boundary of D. The boundary ∂D consists of the four trajectories which converge to the saddle points $\xi = 0$, $\phi = \pm\pi$. Linearizing (6.9) and (6.10) about $\xi = 0$, $\phi = \pm\pi$ we see that δ can be neglected if ε is small and we see that the separating curves are the solutions of (6.9), (6.10) with

$$d\phi/d\xi = \frac{1-\sqrt{3}}{2} \quad \text{at } \xi = 0, \quad \phi = \pm\pi.$$

The expected time between cycle slips is the expected time of first exit from D for the system (6.7), (6.8) where ϕ is taken mod (2π). Thus the expected slip time

$$v(\xi, \phi) = E\{\tau \mid \xi(0) = \xi, \phi(0) = \phi\}$$

is the solution of Dynkin's equation (cf. (3.9))

$$\begin{aligned} L_\varepsilon v &= \varepsilon(v_{\xi\xi} + v_{\xi\phi} + \tfrac{1}{2}v_{\phi\phi}) - (\sin\phi + \delta\xi)v_\xi + (\tfrac{1}{2}\xi - \sin\phi)v_\phi \\ &= -1 \quad \text{in } D, \\ v &= 0 \quad \text{on } \partial D. \end{aligned} \tag{6.11}$$

Since δ is small we neglect the term $\delta\xi v_\xi$. Note that the field in (6.9), (6.10) is not a gradient of a potential, or more precisely, there is no function ψ such that

$$b_j(\xi, \phi) = \sigma_{ij}\psi_\xi + \sigma_{2j}\psi_\phi, \qquad (j = 1, 2)$$

(cf. Matkowsky and Schuss [29]). It follows that the procedure of § 5 has to be modified, since (5.7′) and (5.7″) no longer hold in this case. We proceed as before, scaling v by setting

$$v(\xi, \phi) = C(\varepsilon)\, e^{H/\varepsilon} u(\xi, \phi) \tag{6.12}$$

where H and $C(\varepsilon)$ are constants to be chosen, and $\max u(\xi, \phi) = 1$.

We shall construct a boundary layer expansion for u as in § 5. Let y be the distance from the boundary and let x' be a coordinate in a direction tangent to the boundary. Then the equation for u in the local coordinates (x', y) near ∂D is given by

$$\varepsilon u_{yy} + y b_0(x') u_y + L_1 u = 0, \tag{6.13}$$

where

$$\begin{pmatrix} -\sin\phi \\ \frac{1}{2}\xi - \sin\phi \end{pmatrix} \cdot \boldsymbol{\gamma} = y b_0(x') + O(y^2) \quad \text{as } y \to 0,$$

$\boldsymbol{\gamma}$ = outer normal to ∂D, and $b_0(x')$ is the coefficient of the first term in Taylor's expansion of the function

$$b(x', y) = \begin{pmatrix} -\sin\phi \\ \frac{1}{2}\xi - \sin\phi \end{pmatrix} \cdot \boldsymbol{\gamma}$$

near $y = 0$. We note that $b(x', 0) = 0$ since the vector

$$\begin{pmatrix} -\sin\phi \\ \frac{1}{2}\xi - \sin\phi \end{pmatrix}$$

is tangent to ∂D, by (6.9) and (6.10) (with $\delta - 0$). The expression $L_1 u$ contains tangential and mixed derivatives of u. Setting $\eta = y/\sqrt{\varepsilon}$ we obtain the equation

$$u_{\eta\eta} + \eta b_0(x') u_\eta + L_1 u = 0. \tag{6.14}$$

The second order terms in $L_1 u$ are $O(\sqrt{\varepsilon})$ as $\varepsilon \to 0$. The boundary conditions are

$$u(x', \eta) \to 0 \quad \text{as } \eta \to 0,$$
$$u(x', \eta) \to 1 \quad \text{as } \eta \to \infty.$$

At the points $\xi = 0$, $\phi = \pm\pi$ the first order derivatives in (6.14) vanish. Thus the first term $u^0(x', \eta)$ of the expansion of u near the points $\xi = 0$, $\phi = \pm\pi$ is the solution of the equation

$$u^0_{\eta\eta} + \eta b_0(x') u^0_\eta = 0.$$

Hence

$$u^0(x', \eta) = \int_0^\eta e^{\frac{-s^2 b_0(x')}{2}}\, ds\, b_0^{1/2}(x') / \sqrt{\frac{\pi}{2}}. \tag{6.15}$$

To determine $C(\varepsilon)$ and H we construct a solution $w(\xi, \phi)$ to the adjoint equation

$$L^* w \equiv \varepsilon(w_{\xi\xi} + w_{\xi\phi} + \tfrac{1}{2} w_{\phi\phi}) + \sin\phi w_\xi - [(\tfrac{1}{2}\xi - \sin\phi) w]_\phi = 0,$$

such that $w(0, 0) = 1$. Then, multiplying (6.11) by $w(\xi, \phi)$ and integrating by parts we obtain (Matkowsky and Schuss [29])

$$\begin{aligned} \int_D \int wLv\, d\xi\, d\phi &= \varepsilon \oint_{\partial D} \left[v_\xi \left(\gamma_1 + \frac{1}{2}\gamma_2 \right) + \frac{1}{2} v_\phi (\gamma_1 + \gamma_2) \right] w\, ds \\ &= -\int_D \int w(\xi, \phi)\, d\xi\, d\phi \end{aligned} \tag{6.16}$$

where $\boldsymbol{\gamma} = (\gamma_1, \gamma_2)^T$ is the outer normal at ∂D. We have used here the facts that $v = 0$ on ∂D, and $L^* w = 0$. Inserting (6.12) into (6.15) we obtain

$$C(\varepsilon)\, e^{H/\varepsilon} \oint_{\partial D} \left[u_\xi \left(\gamma_1 + \frac{1}{2}\gamma_2 \right) + \frac{1}{2} u_\phi (\gamma_1 + \gamma_2) \right] w\, ds = -\int_D \int w\, d_\xi\, d\phi. \tag{6.17}$$

We shall construct $w(\xi, \phi)$ using the "ray method" (Cohen and Lewis [7]) and evaluate the integral asymptotically using the Laplace method (Olver [33], [34]) and thus obtain H and $C(\varepsilon)$. We assume that $w(\xi, \phi)$ has the form

$$w(\xi, \phi) = e^{-\Psi(\xi, \phi)/\varepsilon} g(\xi, \phi, \varepsilon), \tag{6.18}$$

where

$$g(\xi, \phi, \varepsilon) \sim \sum_{j=0}^{\infty} g_j(\xi, \phi) \varepsilon^j \tag{6.19}$$

with $\Psi(0, 0) = 0$, $\Psi(\xi, \phi) > 0$ for $\xi^2 + \phi^2 > 0$ and $g_0(0, 0) = 1$. Inserting (6.18) and (6.19) into (6.11) and equating the coefficients of each power of ε separately to zero we obtain equations for ψ and g_j.

In particular Ψ satisfies the nonlinear equation

$$\Psi_\xi^2 + \Psi_\xi \Psi_\phi + \tfrac{1}{2}\Psi_\phi^2 - \sin\phi \Psi_\xi + (\tfrac{1}{2}\xi - \sin\phi)\Psi_\phi = 0 \tag{6.20}$$

while the leading term g_0 in the expansion (6.19) satisfies

$$(6.21)\qquad \begin{aligned}&(2\Psi_\xi+\Psi_\phi-\sin\phi)\partial g_0/\partial\xi+(\Psi_\xi+\Psi_\phi+\tfrac{1}{2}\xi-\sin\phi)\partial g_0/\partial\phi\\&\quad=-(\Psi_{\xi\xi}+\Psi_{\xi\phi}+\tfrac{1}{2}\Psi_{\phi\phi}-\cos\phi)g_0.\end{aligned}$$

Equations (6.20) and (6.21) are equivalent to the following system of six differential equations (Courant and Hilbert [8])

$$(6.22)\qquad \begin{aligned}\dot\xi&=2p+q-\sin\phi\\ \dot\phi&=p+q+\tfrac{1}{2}\xi-\sin\phi\\ \dot p&=-\tfrac{1}{2}q\\ \dot q&=(p+q)\cos\phi\\ \dot\Psi&=p^2+pq+\tfrac{1}{2}q^2\\ \dot g_0&=\chi g_0\end{aligned}$$

where $\chi=-(\Psi_{\xi\xi}+\Psi_{\xi\phi}-\frac{1}{2}\Psi_{\phi\phi}-\cos\phi)$.

Inserting (6.18) into (6.17) and comparing terms of same orders of magnitude in ε we obtain

$$(6.23)\qquad C(\varepsilon)\,e^{H/\varepsilon}\oint_{\partial D}e^{-\Psi/\varepsilon}g_0[u_\xi(\gamma_1+\tfrac{1}{2}\gamma_2)+\tfrac{1}{2}u_\phi(\gamma_1+\gamma_2)]\,ds=-\int_D\int e^{-\Psi/\varepsilon}g_0\,d\xi\,d\phi.$$

Evaluating the Laplace type integrals asymptotically (Olver [33]) we see that the main contribution to the double integral in (6.23) comes from the origin; hence

$$(6.24)\qquad \int\int_D e^{-\Psi/\varepsilon}g_0\,d\xi\,d\phi\approx 2\pi\varepsilon/J$$

where

$$J=\left|\det\begin{bmatrix}\Psi_{\xi\xi}&\Psi_{\xi\phi}\\ \Psi_{\xi\phi}&\Psi_{\phi\phi}\end{bmatrix}\right|\Bigg|_{\xi=0,\phi=0}.$$

The main contribution to the line integral in (6.23) comes from the points of minimum of Ψ on ∂D, namely $\xi=0$, $\phi=\pm\pi$, as follows from the numerical evaluation of Ψ (cf. Fig. 6.4). The asymptotic expansion of the integral about the points $\xi=0$, $\phi=\pm\pi$ is given by

$$(6.25)\qquad \begin{aligned}&\oint_{\partial D}e^{-\Psi/\varepsilon}g_0[u_\xi(\gamma_1+\tfrac{1}{2}\gamma_2)+\tfrac{1}{2}u_\phi(\gamma_1+\gamma_2)]\,ds\\&\quad\approx 2\frac{\sqrt{2\pi\varepsilon}\,e^{-\Psi(0,\pi)/\varepsilon}}{\sqrt{|\Psi''|}}g_0(0,\pi)[u_\xi(\gamma_1+\tfrac{1}{2}\gamma_2)+\tfrac{1}{2}u_\phi(\gamma_1+\gamma_2)]|_{(0,\pi)}\end{aligned}$$

where the factor 2 comes from the invariance of the integrand and ∂D under the transformation $\xi\to-\xi$, $\phi\to-\phi$.

The term Ψ'' is the second derivative of Ψ with respect to arc length in ∂D at $(0,\pi)$. The asymptotic form of $u(\xi,\phi)$ near the point $(0,\pi)$ is given by (6.15), namely

$$u^0(\xi,\phi)\approx b_0^{1/2}(x')\int_0^{y/\sqrt{\varepsilon}}e^{-s^2b_0(x')/2}\,ds\Big/\sqrt{\frac{\pi}{2}};$$

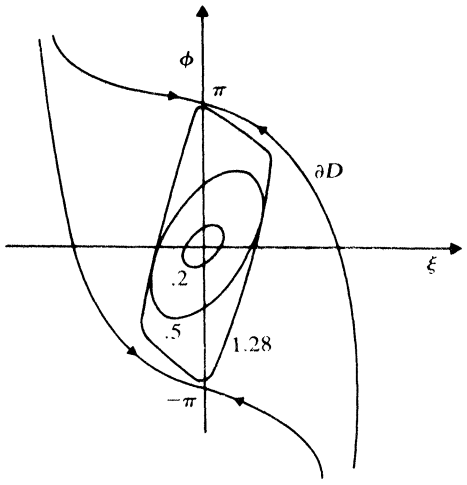

FIG. 6.4. *Level curves of* Ψ.

hence

$$\frac{\partial u^0}{\partial \xi}(0,\pi) = b_0^{1/2}(0)\frac{\partial y}{\partial \xi}\Big/\sqrt{\frac{\pi\varepsilon}{2}}\Big|_{\xi=0,\phi=\pi}$$

$$= b_0^{1/2}(0)\frac{1-\sqrt{3}}{2}\Big/\left\{\frac{\pi\varepsilon}{2}\left[1+\left(\frac{1-\sqrt{3}}{2}\right)^2\right]\right\}^{1/2},$$

$$\frac{\partial u^0}{\partial \phi}(0,\pi) = -b_0^{1/2}(0)\Big/\left\{\frac{\pi\varepsilon}{2}\left[1+\left(\frac{1-\sqrt{3}}{2}\right)^2\right]\right\}^{1/2}.$$

Thus

$$u_\xi^0(\gamma_1+\tfrac{1}{2}\gamma_2)+\tfrac{1}{2}u_\phi^0(\gamma_1+\gamma_2)|_{\xi=0,\phi=\pi}$$

$$= -b_0^{1/2}(0)\Big/\left[\left[\frac{4-\sqrt{3}}{2}\right]\sqrt{\frac{\pi\varepsilon}{2}}\right] = -\frac{\sqrt{3}+1/\sqrt{3}}{\sqrt{\frac{\pi\varepsilon}{2}}\,\frac{4-\sqrt{3}}{2}}.$$

Now, linearizing the coefficients of (6.20) near $\xi = 0$, $\phi = \pi$ and using Taylor's expansion of Ψ about this point we obtain

$$\Psi = \Psi(0,\pi) - \xi(\phi-\pi) + O(\xi^2+(\phi-\pi)^2).$$

Hence

$$|\Psi''| = \frac{\sqrt{3}-1}{4-\sqrt{3}}.$$

The boundary integral (6.25) is therefore equal to $-13.725\, g_0(0,\pi)$ $\exp[-\Psi(0,\pi)/\varepsilon]$. Substituting this last expression and (6.24) in (6.23) we obtain

$$13.725C(\varepsilon)\, e^{H/\varepsilon} g_0(0,\pi)\, e^{-\Psi(0,\pi)/\varepsilon} = 2\pi/J.$$

Using Taylor's expansion of $\Psi(\xi, \phi)$ about $\xi = 0, \phi = \pi$ we find that

$$\Psi = \tfrac{1}{2}\xi^2 - \xi\phi + \phi^2 + O(\xi^2 + \phi^2);$$

hence $J = 1$. It follows that $H = \Psi(0, \pi)$ and $C(\varepsilon) = 2\pi/[13.725 g_0(0, \pi)]$; hence

$$v(0, 0) \approx \frac{2\pi e^{\Psi(0,\pi)/\varepsilon}}{13.725 g_0(0, \pi)}$$

or

$$kE(\tau \mid \xi(0) = 0, \phi(0) = 0) = \frac{2\pi\Lambda^{-1/4}}{13.725\, g_0(0, \pi)\sqrt{2\beta}} \exp\left[\frac{\Psi(0, \pi)}{2\sqrt{2\beta}}\Lambda^{3/4}\right] \tag{6.26}$$

where $\Psi(0, \pi) \approx 1.28$ and $g_0(0, \pi) \approx e^{-4}$.

In most practical cases one presently finds PLL's with constant gains i.e. gains independent of Λ. Such loops were extensively studied for randomly modulated signals, i.e. for $x(t)$ = random process (Lindsey [24], Van Trees [46], Viterbi [49]). However no results concerning $E\tau$ in this case are given there. Such loops lead to regular perturbation problems in N_0. If the gains of such loops are chosen according to practical considerations one can nevertheless obtain a problem with two small parameters, λ and N_0, where λ is a design parameter. A similar method shows that

$$E\tau\alpha \exp\left[\Psi(0, \pi)\Lambda^{3/4}/(\lambda\Lambda^{3/4} + 2\sqrt{2\beta})\right], \tag{6.27}$$

where $.2 \leqq \lambda \leqq .25$. If $\Lambda \to \infty$ then $E\tau \to$ const. $< \infty$, unlike the variable gain case of (6.28) (cf. Fig. 6.5 below)

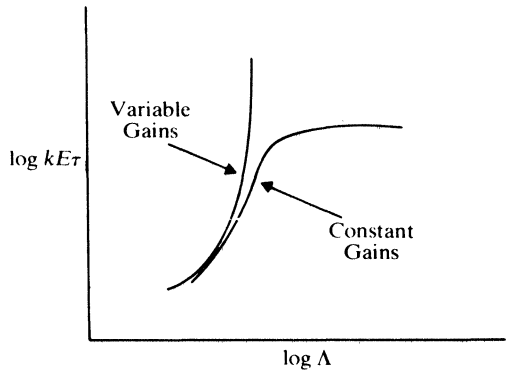

FIG. 6.5. $E\tau$ *for constant and variable gains.*

7. First passage problems in mechanical systems and electric networks. Consider the equations of motion of an elastic system expressed by generalized coordinates $q_1(t), \cdots, q_n(t)$

$$\rho_j\ddot{q}_j + 2\eta_j\dot{q}_j + f_j(q_1, \cdots, q_n) = \gamma_j(t) \qquad (j = 1, 2, \cdots, n). \tag{7.1}$$

Here ρ_j are inertia coefficients, η_j are damping coefficients, f_j are some nonlinear functions of the coordinates q_i. We shall assume that the system is driven by white noise γ_j so that

$$E\gamma_j(t) = 0, \qquad E\gamma_j(t)\gamma_k(t + s) = c_{jk}\delta(s)$$

where c_{jk} are some constants.

To write down the Fokker–Planck equation corresponding to the system (7.1) we rewrite the system in the Itô form first. The white noises $\gamma_j(t)$ $(j=1,\cdots,n)$ can be represented by

$$\gamma_i(t)\,dt=\sum_{j=1}^{n}a_{ij}\,dw_j(t)$$

where $\sum_{l=1}^{n}a_{jl}a_{kl}=c_{jk}$, and where $w_j(t)$ are independent Brownian motions. Setting

$$\mathbf{x}=\mathbf{q},\qquad \mathbf{y}=\dot{\mathbf{q}}$$

we have, by (7.1)

$$d\mathbf{x}=\mathbf{y}\,dt,$$

$$\mathbf{R}\,d\mathbf{y}=-(2\boldsymbol{\Psi}\mathbf{y}+\mathbf{f}(\mathbf{x}))\,dt+\mathbf{A}\,d\mathbf{w},$$

where

$$\mathbf{R}_{ij}=\rho_j\delta_{ij},\quad \boldsymbol{\Psi}_{ij}=\eta_j\delta_{ij},\quad \mathbf{f}_j(\mathbf{x})=\mathbf{f}_j(q_1,\cdots,q_n)$$

and $\mathbf{A}_{ij}=a_{ij}$. The Fokker–Planck equation for (7.1) is now given by

$$p_t=-\sum_{i=1}^{n}\dot{q}_ip_{q_i}+\sum_{j=1}^{n}\frac{2\eta_j}{\rho_j}(p+\dot{q}_jp_{\dot{q}_j})+\sum_{j=1}^{n}\frac{1}{\rho_j}\,(pf_j)_{\dot{q}_j}+\frac{1}{2}\sum_{j,k=1}^{n}\frac{c_{jk}}{\rho_j\rho_k}p_{\dot{q}_j\dot{q}_k},$$

where $p_t=\partial p/\partial t$, etc. The function

$$p=p(\mathbf{q}_0,\dot{\mathbf{q}}_0,\mathbf{q},\dot{\mathbf{q}},t)$$

satisfies the initial condition

$$p\to\delta(\mathbf{q}-\mathbf{q}_0,\dot{\mathbf{q}}-\dot{\mathbf{q}}_0)\quad\text{as } t\downarrow 0.$$

It represents the transition probability density of the system in phase space. If $f_j=-(1/\rho_j)U_{q_j}$, then (7.1) has stable equilibrium points at local minima of U. A neighborhood of a stable equilibrium point in phase space, which is permissible from normal functioning point of view is called a "reliability region". This region may be the elasticity region of the system, a limit on the total energy of the system set by safety requirements etc. The probability density of the exit points is the probability of failure of a given component of the system. Equation (3.11) for the expected failure time is given by

$$\sum_{i,j=1}^{n}\sigma_{ij}\frac{\partial^2 v}{\partial y_i\partial y_j}-2\sum_{j=1}^{n}\frac{\eta_j}{\rho_j}\frac{\partial v}{\partial y_j}-\sum_{j=1}^{n}\frac{f_j}{\rho_j}\frac{\partial v}{\partial x_j}=-1 \tag{7.2}$$

in the domain of reliability Ω and $v=0$ on $\partial\Omega$. Here, by (3.10)

$$\sigma_{ij}=\tfrac{1}{2}c_{ij}/\rho_i\rho_j,\qquad (i,j=1,\cdots,n)$$

(cf. Bolotin [4]).

The differential equation corresponding to the simplest model of a thin elastic curved panel is

$$\rho\ddot{x}+2\eta\dot{x}+\rho\omega^2 f(x)=\gamma(t). \tag{7.3}$$

Here $x(t)$ is the deflection of the panel, $\rho=$ inertia coefficient, $\eta=$ damping coefficient, $\omega=$ natural frequency,

$$f(x)=-U'(x)$$

where $U(x)$ has two or more minima. The passage of the system from one stable equilibrium to another is called "dynamical snap-through". This phenomenon requires the passage of the system through an unstable equilibrium point. We will consider the system snapped through if its energy suffices to move it over the potential barrier when $\gamma \equiv 0$, $\eta = 0$. If the graph of U is given as in Fig. 7.1

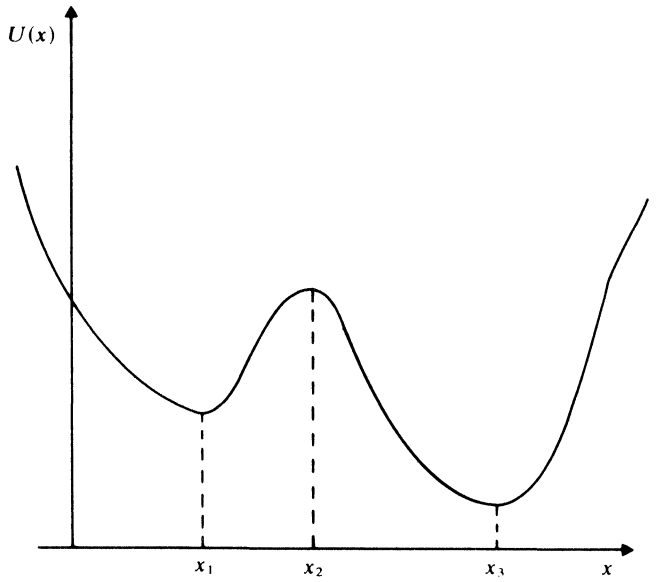

FIG. 7.1. *The potential for the dynamical snap through.*

and x_1 is the initial state, then x_3 is the snapped through state, x_2 is the barrier and the domain

$$E(x, \dot{x}) = \frac{\rho \dot{x}^2}{2} + \rho\omega^2 U(x) < \rho\omega^2 U(x_2), \qquad (x < x_2)$$

is the permissible region. The boundary $\partial\Omega$ is the separatrix (cf. Fig. 7.2)

$$\frac{\rho \dot{x}^2}{2} + \rho\omega^2 U(x) = \rho\omega^2 U(x_2).$$

The reliability problem is to find the expected time until $E = \rho\omega^2 U(x_2)$. We have

$$\frac{a}{2\rho^2} v_{yy} + y v_x - \omega^2 f(x) v_y - \frac{2\eta}{\rho} v_y = -1 \quad \text{in } \Omega$$

$$v = 0 \quad \text{on } \partial\Omega.$$

If $\varepsilon = a/(2p^2) \ll 1$ then the methods of § 3 can be used to obtain asymptotic solutions (cf. Bolotin [5]).

A more realistic model is a system consisting of two rigid bars of length $l/2$ and two elastic hinges (cf. Slemrod [43]). It is taken as an approximation of a real deformable beam. Assume the load P is to follow the deflections (a "follower load", Bolotin [4]). ϕ_i are the deflection angles of the bars, C_i are elastic constants of the hinges, m_i are the masses of the bars fixed at distances αl and γl, β is a damping coefficient. The linearized

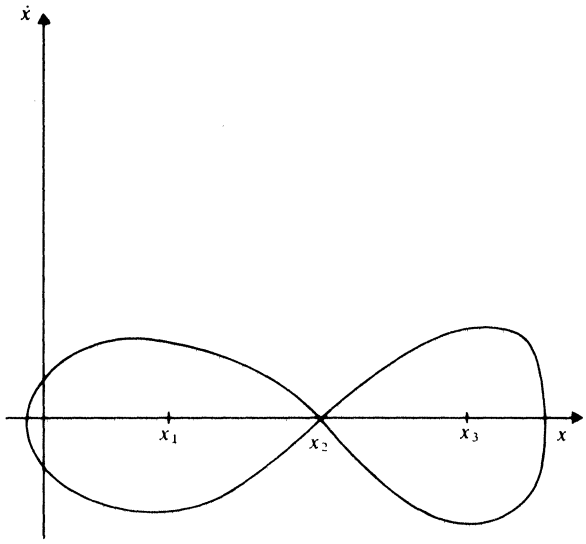

FIG. 7.2. *The separatrix for the dynamical snap through.*

equations of motion are

$$\mathbf{M}\ddot{\mathbf{x}} + \beta\dot{\mathbf{x}} + (\mathbf{C}+\mathbf{D})\mathbf{x} = 0$$

$$\mathbf{x} = \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}$$

$$\mathbf{M} = \begin{bmatrix} (m_1^2 + \frac{1}{4}m_2(l^2) & \frac{1}{2}m_2\gamma l^2 \\ \frac{1}{2}m_2 l^2\gamma & m_2\gamma^2 l^2 \end{bmatrix}$$

$$\mathbf{C} = \begin{bmatrix} C_1 + C_2 & -C_2 \\ -C_2 & C_2 \end{bmatrix}$$

$$\mathbf{D} = \begin{bmatrix} -\frac{1}{2}P(t)l & \frac{1}{2}P(t)l \\ 0 & 0 \end{bmatrix}$$

(cf. Fig. 7.3). It is known that if $P < P_C$ = critical load, the double pendulum is Lyapunov stable. If $P = P_0(1+\gamma)$ where γ is white noise we obtain a stochastic system of the form

$$d\mathbf{y} = \mathbf{A}\mathbf{y}\,dt + \mathbf{B}\mathbf{y}\,dw$$

where

$$\mathbf{y} = \begin{pmatrix} \mathbf{x} \\ \dot{\mathbf{x}} \end{pmatrix}$$

A and **B** are constant matrices such that the eigenvalues of **A** are purely imaginary if $\beta = 0$, otherwise the eigenvalues have negative real parts, and

$$\mathbf{B} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ -\mathbf{H} & \mathbf{0} \end{pmatrix}, \qquad \mathbf{H} = \tfrac{1}{2}l\mathbf{M}^{-1}\begin{pmatrix} -1 & 1 \\ 0 & 0 \end{pmatrix}.$$

The backward Kolmogorov equation is given by

$$\sum_{i,j,k,l=1}^{4} a_{ijkl}y_k y_l p_{y_i y_j} + \mathbf{A}\mathbf{y}\cdot\nabla_{\mathbf{y}}p = p_t. \tag{7.4}$$

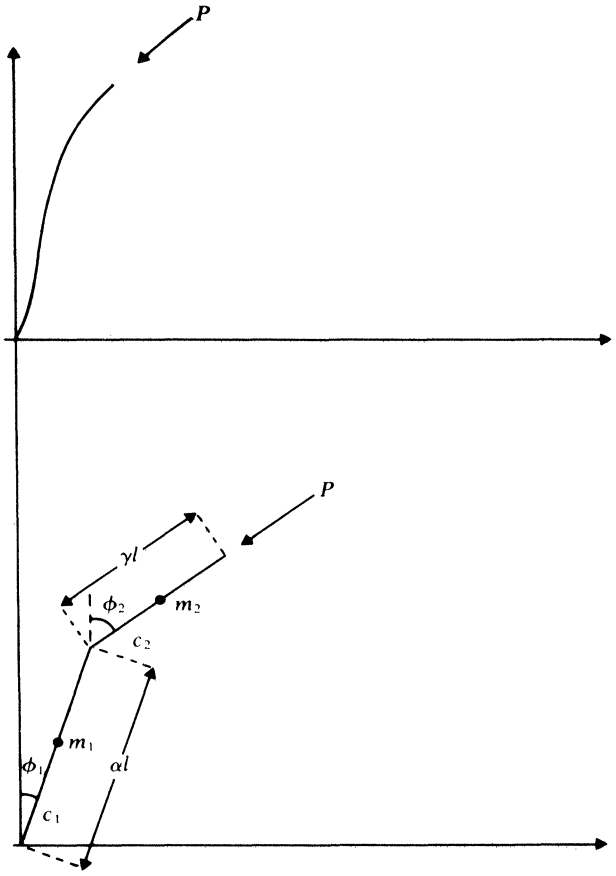

FIG. 7.3. *Elastic beam with a follower load.*

The function $p = p(\mathbf{y}_0, t, \mathbf{y})$ is the transition probability density. The matrix is given by

$$A = \begin{bmatrix} 0 & I \\ \mathbf{M}^{-1}(\mathbf{C}+\mathbf{D}_0) & -\beta\mathbf{M}^{-1} \end{bmatrix}$$

and $a_{ijkl} = \mathbf{B}_{ik}\mathbf{B}_{jl}$, $\mathbf{D}_0$ is the matrix $\mathbf{D}$ with $P(t) = P_0$.

Equation (7.4) is a degenerate parabolic equation. The reliability problem is the same as in the previous example. The stability of the system was investigated by Parthasarathy and Evan-Iwanowski [38]. A similar degenerate parabolic problem arises in electric networks subjected to random (e.g. thermal) e.m.f. A complete description of such a problem is given in Wang and Uhlenbeck [50]. Further problems of first passage in electric circuits are given in Stratonovich [45].

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