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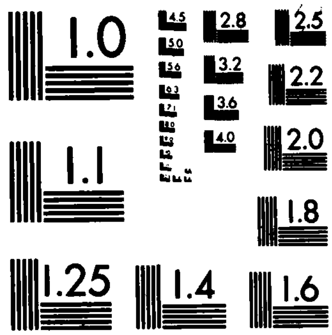

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Under this grant, was supported a successful collaboration between Professors B.J. Matkowsky, Z. Schuss, and S. Kamin on Singular Perturbation scientific disciplines. The effects of random (stochastic) perturbations on deterministic dynamical system were considered including (1) the effects of noise on deterministic dynamics (such noise exists in all physical systems), and (2) specific physical effects, the details of which are very complicated, and are modeled as stochastic terms.

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FINAL REPORT

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AFOSR 78-3602[redacted]

"FIRST PASSAGE TIMES IN STOCHASTIC DIFFERENTIAL EQUATIONS OF MATHEMATICAL PHYSICS AND ENGINEERING"

Principal Investigator

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May 1983

Final Report

Air Force Office of Scientific Research Grant AFOSR 78-3602A,B,C,D, entitled "First Passage Times in Stochastic Differential Equations of Mathematical Physics and Engineering"

Principal Investigator: Prof. Bernard J. Matkowsky
Department of Engineering Sciences and Applied Mathematics
The Technological Institute
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Under this grant, we supported the successful collaboration between Professors B. J. Matkowsky, Z. Schuss, and S. Kamin on Singular Perturbation Methods in Stochastic Differential Equations and Applications to various scientific disciplines. We made a number of breakthroughs on some fundamental problems, both in science and in mathematics.

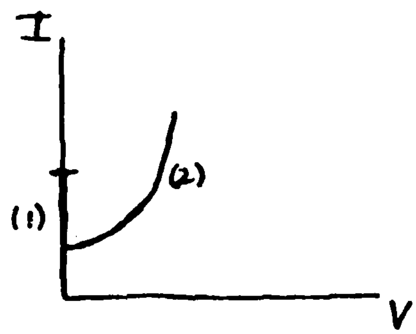
We considered the effects of random (stochastic) perturbations on deterministic dynamical systems, including (i) the effects of noise on deterministic dynamics (such noise exists in all physical systems), and (ii) specific physical effects, the details of which are very complicated, and are modeled as stochastic terms; e.g. (a) the effect of molecular collisions which causes chemical reactions and (b) the effect of random thermal vibrations of a crystal lattice which causes diffusion. With the inclusion of random perturbations, the deterministic differential equations become stochastic differential equations. The effects of random perturbations include (i) fluctuations about stable steady state solutions of the deterministic dynamics, and (ii) jumps or transitions from one stable state to another.

The distribution of fluctuations about stable equilibrium solutions is given by the Boltzmann distribution $\rho \sim e^{-E/T}$, where E denotes energy and T denotes temperature. For fluctuations about stable non-equilibrium solutions (such as limit cycles), our results are new. They are of the form $\rho \sim \rho_0 e^{-W/T}$ where W plays the role of energy, is a solution of a Hamilton-Jacobi type equation, which we derive. The fact that such jumps or transitions occur, can be used as the basis of explanations of various scientific phenomena: e.g. ionic conductivity in crystals and chemical reactions. In addition it can be used as the basis for studying the relative stability of two or more (meta)stable states in a multi-stable system.

We introduced new mathematical methods to compute (i) the distribution of fluctuations about stable steady state solutions of the deterministic dynamics, and (ii) the transition rate (jump frequency) from one stable state to another. The transition rate from a stable state is inversely proportional to the lifetime of (first passage time from) that state. This allowed us to compute the relative stability of a stable state in a system in which there exist multiple stable states. The state with a longer lifetime is considered to be more stable.

The lifetimes of stable equilibrium states of potential systems, is proportional to the height of the potential barrier which must be overcome, in order for a transition to occur. For the lifetimes of stable non-equilibrium states our results are again new. The analog of the barrier height is a critical value of the function W described above, which we compute.

<u>example</u>: The Josephson junction is to be employed as a logical element (switch) in the next generation of computers. It has two stable solutions. (1) - The superconducting solution in which the current I ≠ 0, but the voltage V = 0, and (2) - a solution with both I and V ≠ 0.



solution (1) with V = 0, corresponds to off (or No)
solution (2) with V ≠ 0 corresponds to on (or Yes)

To determine the reliability of this element, it is important to know the frequency of jumps due to noise from one solution to another. Our methods compute such jump frequencies.

Our approach was to characterize the quantities of interest as solutions of singularity perturbed elliptic boundary value problems, which are obtained from the stochastic differential equations via the Ito calculus. We then introduced new perturbation methods to solve the singularity perturbed boundary value problems. In addition to computing (explicitly analytically) the desired quantities, we obtained as a by-product, extensions of the Method of Averaging, and of the method of Matched Asymptotic Expansions.

In summary the research produced during the four year period of the grant, has been most successful. During that period 20 papers and one book have been published. They are summarized below:

Book: Theory and Applications of Stochastic Differential Equations, J. Wiley, (1980), New York.

Research Papers

1. "The exit problem: a new approach to diffusion across potential barriers," SIAM J. Appl. Math., 35 (1979), pp. 604-623.

   We consider the problem of a Brownian particle confined in a potential well of forces, which escapes the potential barrier as the result of white noise forces acting on it. The problem is characterized by a diffusion process in a force field and is described by Langevin's stochastic differential equation. We consider potential wells with many transition states and compute the expected exit time of the particle from the well as well as the probability distribution of the exit points. Our method relates these quantities to the solutions of certain singularly perturbed elliptic boundary value problems which are solved asymptotically. Our results are then applied to the calculation of of chemical reaction rates by considering the breaking of chemical bonds caused by random molecular collisions, and to the calculation of the diffusion matrix in crystals by considering random atomic migration in the period force field of the crystal lattice, caused by thermal vibration of the lattice.

2. "On elliptic singular perturbation problems with turning points," SIAM J. Appl. Math., 10 (1979), pp. 447-455.

   The boundary value problem for the elliptic equation $\varepsilon\Delta u + \sum b_i u_{x_i} = 0$ is considered in the case that the characteristic curves of the reduced equation enter the domain and have a singular point inside (turning point). Assume that there exists a potential function $\psi(x)$ such that $b_i = \psi_{x_i}$ $(i=1,2,\cdots,n)$. It is proved that if $\varepsilon \to 0$ then the solutions $u_\varepsilon(x)$ converge to a constant, a formula for which was derived by Matkowsky and Schuss using formal asymptotic expansion.

3. "Eigenvalues of the Fokker-Planck operator and the approach to equilibrium for diffusion in potential fields," SIAM J. Appl. Math., 40 (1981), pp. 242-254.

   We consider the motion of a Brownian particle in an infinite potential field. The rate of approach to equilibrium is determined by the second eigenvalue of the stationary Fokker-Planck operator. The inverse of this eigenvalue is the expected time for the particle to overcome the potential barriers on its way to the deepest potential well. The height of the largest potential barrier is termed the activation energy, and the eigenvalue is computed asymptotically for large activation energies. Applications to the calculation of chemical reaction rates and ionic conductance in crystals are given.

4. "Singular Perturbations, Stochastic Differential Equations and Applications," in Singular Perturbations and Asymptotics, ed. R. E. Meyer and S. V. Parter, Academic Press, New York, 1980.

   Invited address at the Advanced Seminar on Singular Perturbations and Asymptotics, in honor of W. Wasow, held at the University of Wisconsin, Madison, May 1980.

5. "Thermal fluctuations and lifetime of the nonequilibrium state in a hysteretic Josephson junction," Phys. Rev. B25 (1982), pp. 519-522.

   The probability distribution of thermal fluctuations around the finite-voltage steady state of a hysteretic Josephson junction, as well as the transition probability out of that state, are both calculated by a simple method that promises to be applicable to a wide variety of nonequilibrium steady-state situations. Our results are in excellent agreement with those obtained by numerical simulations. Specific experiments are suggested in order to verify the results for the Josephson junction.

6. "The mean lifetime of meta-stable states of the DC-SQUID and its I-V characteristics,". National Bureau of Standards Special Publication 614. Sixth Int'l Conf. on Noise in Physical Systems (1981), 376-380.

   The DC-SQUID with small coupling has several types of meta-stable states and therefore it can be used as a logic element. At a finite temperature the thermal noise causes spontaneous transitions between the various states. Hence, the meta-stable states have finite mean lifetimes. It is of interest to know the dependence of these lifetimes on the DC-SQUID parameters, on the external driving current I and on the external magnetic flux Φ_{ex}. Here we find this dependence for the shunted DC-SQUID.

7. "Kramers' diffusion problem and diffusion across characteristic boundaries," in Theory and Applications of Singular Perturbations, Conf. Proceedings, Oberwolfach, 1981, pp. 318-345, Ed. W. Eckhaus and E. M. de Jager, Spring Lectures Notes in Mathematics, No. 942, (invited address).

8. "Diffusion across characteristic boundaries," SIAM J. Appl. Math., 42 (1982), pp. 822-834.

   We consider the motion of a particle acted on by the deterministic force vector b(x(t)) and perturbed by random forces of white noise type. Such a particle will leave any bounded domain Ω in finite time. We consider the case where b is such that $\partial\Omega$ consists of a trajectory or trajectories of the system $x = b(x(t))$. Thus we consider the cases of an unstable limit cycle and a center. We observe that these problems are such that b is not derivable from a potential. For each problem we derive expressions for (i) the mean first passage time to $\partial\Omega$, and (ii) the probability distribution of exit points on $\partial\Omega$. Our method is to employ the Ito calculus to characterize the quantities (i) and

(ii) as solutions of singularly perturbed elliptic boundary value problems, and then to derive asymptotic representations of the solutions of those problems. The results obtained are new and are of importance in a variety of applications including the estimation of jump times (due to noise) from stable periodic solutions to other stable solutions of the deterministic dynamical system.

9. "A singular perturbation approach to Kramers' diffusion problem," SIAM J. Appl. Math., 42 (1982), pp. 835-849.

We consider Kramers' diffusion problem, which seeks to calculate the rate of escape of a particle from one potential well over a barrier, to another presumably deeper and therefore more stable well. Though Kramers introduced the problem as a model for chemical reactions, it applies to numerous rate processes, including atomic migration and ionic conductivity in crystals, and transitions due to noise, between stable states of dynamical systems with multi-stable states, to name but a few. We propose a new approach, not based on a Fokker-Planck equation, but rather on the solution of a singularly perturbed boundary value problem. Specifically, we relate the rate of escape to the first passage time from the domain of attraction of the stable point corresponding to the first well. The first passage time is then characterized via the Ito calculus, as a solution of an elliptic partial differential equation of singular perturbation type. Finally this equation is solved asymptotically by methods previously developed by the authors. We obtain some new results on the rate of escape, which reduce to those of Kramers for the cases he considered, and in addition discuss the validity of the various results derived by Kramers. Finally, in contrast to other approaches, our methods readily extend to higher dimensions.

10. "A singular perturbation method for the computation of the mean first passage time in a nonlinear filter," SIAM J. Appl. Math., 42 (1982), pp. 174-187.

We give a new application of recently developed singular perturbation methods in the area of mathematical theory of nonlinear filtering. We consider the phenomenon of cycle slipping in a second order phase-locked loop (PLL) which serves as demodulator for a random FM message. We introduce new scaling parameters into the Ito system of stochastic differential equations describing the PLL, thus identifying the phenomenon of cycle slipping with Kolmogorov's exit problem. We use singular perturbation methods to obtain an explicit expression for the mean time between cycle slips. Furthermore, we sescribe the mechanism of cycle slips and identify new parameters which determine the probability of their occurrence.

11. "Dynamical systems driven by small white noise: asymptotic analysis and applications," survey paper to appear as a chapter in forthcoming Springer-Verlag book on Singular Perturbations and Asymptotics, ed. by F. ver Hulst.

12. "Diffusion across characteristic boundaries with critical points," SIAM J. Appl. Math., 43 (1983).

    We consider the problem of the effect of small white noise perturbations on a deterministic dynamical system in the plane with (i) an asymptotically stable equilibrium point or limit cycle and (ii0 an equilibrium point surrounded by closed trajectories. The mean exit time and the distribution of exit points for each problem is determined by solving singularly perturbed elliptic boundary value problems in domains with closed characteristic boundaries with critical points. Uniformly valid asymptotic solutions are constructed for each of the problems. For the asymptotically stable equilibrium point, the method of matched asymptotic expansions with the integral condition of Matkowsky and Schuss is employed. A method of averaging combined with boundary layer analysis is used for the problem of an equilibrium point surrounded by closed trajectories. The influence on the solutions, of the critical points on the boundary, is exhibited and explained. An application to the physical pendulum is given. Finally our results are shown to be in close agreement with simulations.

13. "Thermal and shot noise effects on nonlinear oscillators," to appear in Annals of New York Academy of Sciences. Proceedings of 5th Int'l Conf. on Collective Phenomena, Moscow.

14. "On singular perturbation problems with several turning points," Indiana Univ. Math. J., 31 (1982), pp. 819-841.

    Provides rigorous proofs for the results in reference 1.

15. "Lifetime of oscillatory steady states," Phys. Rev. A., 26 (1982), pp. 2806-2816.

    We introduce a method to derive expressions for the distribution ρ of large fluctuations about a stable oscillatory steady state and for the transition rate from that state into another stable state. Our method is based on a WKB-type expansion of the solution of the Fokker-Planck equation. The expression for ρ has a form similar to the Boltzmann distribution with the energy replaced by a function W, which is the solution of a Hamilton-Jacobi-type equation. For the case of small dissipation, a simple analytical approximation to W, in terms of an action increment, is derived. Our results are employed to predict various measurable quantities in physical systems. Specifically we consider the problems of the physical pendulum, the shunted Josephson junction, and the transport of charge-density-wave excitations.

16. "On the lifetime of a metastable state at low noise," accepted, Physics Letters (1983).

    The mean lifetime of a metastable state of a dynamical system driven by small white noise is calculated. The vector field of the dynamical system which need not be deriveable from a potential, is assumed to have a vanishing normal component on the boundary of the domain of attraction of the metastable state.

17. "Transitions from the equilibrium state of a hysteretic Josephson junction induced self-generated shot noise," submitted, Phys. Rev. Letters.

We postulate the existence of self-generated normal current shot noise due to the long-lived voltage fluctuations in a hysteretic Josephson junction. The resulting low temperature transition rates out of the (zero voltage) superconducting state are much larger than those arising from Johnson noise alone. Excellent agreement with experiments is then achieved at all temperatures, removing the need to invoke macroscopic quantum tunneling.

18. "Shot noise effect on the nonzero voltage state of the hysteretic Josephson junction," accepted, Applied Phys. Letters (1983).

We find a non-symmetric distribution of voltage fluctuations about the nonzero voltage state of a hysteretic Josephson junction when shot noise effects are included. The positive voltage fluctuations are found to be more probable than the negative ones. We also find that the transition rates become larger than those due to Johnson noise only.

19. "Thermal activation from the fluxoid and the voltage states of DC-SQUIDS," accepted, J. Applied Physics (1983).

The probability density of thermal fluctuations about different types of nonequilibrium steady states of a DC-SQUID are evaluated by generalizing a technique used before for the fluctuations of a single Josephson junction. Probability densities obtained for both "running" and "beating" modes are used to calculate thermal activation rates as well as the various branches of the I-V characteristic. The results are compared with the experiments of Voss et al. and good agreement is found.

20. "Asymptotic analysis of the optimal filtering problem for one dimensional diffusion measured in a low noise channel I," to appear, SIAM J. Appl. Math.

We consider the problem of filtering a diffusion with nonlinear drift transmitted through a linear low noise channel. A ray method is used for the construction of approximate solutions to Kushner's and Zakai's equations for the normalized and unnormalized conditional probability density function of the signal. A systematic expansion of the mean square estimation error is given, the realization of an asymptotic optimal filter is presented and shown to be one dimensional. Some examples are worked out and the relation to some recent work of Beneš and Hijab is discussed.