

# Analytical And Numerical Study Of Kramers' Exit Problem II \*

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## Abstract

Kramers' exit problem is concerned with noise activated escape from a potential well. In case the noise strength,  $\epsilon$ , (temperature measured in units of potential barrier height) is small this becomes a singular perturbation problem. It is shown that actually, most of the probability of the exit points on the separatrix is located at a distance  $O(\sqrt{\epsilon})$  from the saddle point and the probability vanishes altogether at the saddle point. The stochastic dynamics of the escaping trajectories, conditioned on not returning to a given critical energy contour, are studied analytically and numerically.

## 1 Introduction

This paper continues the research started in "Analytical and Numerical Study of Kramers' Exit Problem I" (see [1]). We remind the reader that the main purpose of this work is to give a complete description of the exit distribution in the Kramers problem which is concerned with the motion of a Brownian particle in a field of force. The motion is described by the dimensionless Langevin equation

$$\ddot{x} + \beta\dot{x} + U'(x) = \sqrt{2\epsilon\beta}\dot{w}, \quad (1)$$

where  $U(x)$  is a potential that forms a well with barrier height normalized to 1,  $\beta$  is the dissipation constant, normalized by the frequency of vibration at the bottom of the well,  $\epsilon$  is dimensionless temperature, normalized by the barrier height, and  $\dot{w}$  is standard Gaussian white noise [2]. If  $\epsilon$  is a small parameter (e.g., if the barrier of the well is high), the stochastic trajectories of eq.(1) stay inside the well for a long time, but ultimately escape [2].

To describe the escape process the Langevin equation is converted to the phase plane system

$$\begin{aligned} \dot{x} &= y \\ \dot{y} &= -\beta y - U'(x) + \sqrt{2\epsilon\beta}\dot{w}. \end{aligned} \quad (2)$$

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The domain of attraction of the stable equilibrium point of the noiseless dynamics,

$$\begin{aligned}\dot{x} &= y \\ \dot{y} &= -\beta y - U'(x),\end{aligned}\tag{3}$$

located at the bottom of the potential well, is denoted by  $D$  and is bounded by a separatrix,  $\Gamma$ , that is, the locus of points where the random trajectories of (2) are equally likely to escape or to return to the well (see Figure 1.1). Here the potential  $U$  is given by  $U(x) = 2x^4 - 1.2x^3 - 2x^2 + 1.45$ , and the dissipation constant  $\beta = 2$ . The plotting process was done with the help of the MATLAB program. The specific exit problem for (2) is to determine the probability density function (pdf) of the points where escaping trajectories hit  $\Gamma$ .

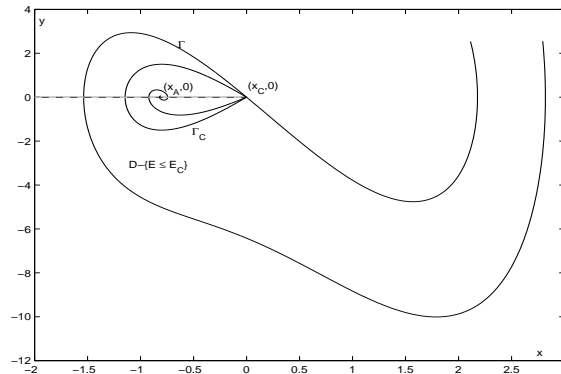


Fig. 1.1. The domain of attraction  $D$  is bounded by the separatrix  $\Gamma$ .

The domain  $D = \{E \leq E_C\}$  is bounded between  $\Gamma$  and by the critical energy contour  $\Gamma_C$ .

This is achieved by mapping the exit distribution on the critical energy contour onto the separatrix, as found in [3], by means of the tails of the escaping trajectories. The tails, which are the trajectories of the original dynamics conditioned on reaching the separatrix before returning to the critical energy contour, obey different dynamics than the original trajectories [4]. The idea of conditioning was proposed in [4] and used in [5] for elucidating some of the features of the phenomenon of saddle point avoidance. The application of the method of conditioning to Kramers' problem requires separate analysis because the noise matrix is degenerate. We construct a boundary layer for the solution of the Fokker-Planck equation of the conditioned dynamics and match it with the outer solution. The numerical study of the noiseless conditioned dynamics reveals the peculiar behavior of the escaping trajectories near the separatrix. The tails of the escaping trajectories tend to move in the opposite direction to that of the original dynamics and aggregate near a point on the separatrix removed a distance of  $O(\sqrt{\epsilon})$  away from the saddle point.

Our main results are the uniform leading order asymptotic expansion of the solution of the stationary Fokker-Planck equation for the pdf of the tails, and an asymptotic expansion of the pdf of their exit points on  $\Gamma$ , in the limit of small  $\epsilon$ . We give a numerical and graphical representation of the important components of the asymptotic solution and also compare the graph of the expression for the exit pdf with a normalized

histogram of exit points obtained by numerical simulation of the original stochastic dynamics (2). The result indicates that this pdf is asymmetric about its maximum which is achieved at a point on  $\Gamma$  whose distance from the saddle point is  $O(\sqrt{\epsilon})$ .

## 2 Previous results

A trajectory that crosses  $\Gamma_C$  goes on to cross  $\Gamma$  and escape the domain of attraction  $D$ . The part of an escaping trajectory from the last point where it hits  $\Gamma_C$  to the first point it hits  $\Gamma$  is referred to as *the tail* of the escaping trajectory. To investigate the problem of escape, we track the tails of the escaping trajectories.

The tails of the escaping trajectories form a new diffusion process, denoted by  $(x^*(t), y^*(t))$ , and defined in the domain  $D - \{E \leq E_C\}$ , enclosed between  $\Gamma_C$  and  $\Gamma$ . This process has the same noise matrix as the original one and drift vector

$$\mathbf{b}^*(x, y) = \begin{pmatrix} y \\ -\beta y - U'(x) + 2\epsilon\beta \frac{\partial \ln P(x, y)}{\partial y} \end{pmatrix}. \quad (4)$$

That means

$$\begin{aligned} \dot{x}^*(t) &= y^*(t) \\ \dot{y}^*(t) &= -\beta y^*(t) - U'(x^*(t)) + 2\epsilon\beta \frac{\partial \ln P(x^*(t), y^*(t))}{\partial y} + \sqrt{2\epsilon\beta} \dot{w}. \end{aligned} \quad (5)$$

Note that the first component of the new drift is the same as that of the original drift, but the second component has the additional term  $2\epsilon\beta \partial \ln P(x, y) / \partial y$ .

The function  $P(x, y)$  is the solution of the backward Kolmogorov equation [7] in the domain  $D - \{E \leq E_C\}$ , with the boundary conditions

$$P(x, y_\Gamma(x)) = 1, \quad P(x, y_C(x)) = 0. \quad (6)$$

We transformed  $P(x, y)$  to the form  $P(x, y) = \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\chi(x, y)/\sqrt{\epsilon}} e^{-z^2/2} dz$ , where the function  $\chi(x, y)$  satisfies the equation

$$y \frac{\partial \chi(x, y)}{\partial x} - [\beta y + U'(x)] \frac{\partial \chi(x, y)}{\partial y} = \beta \left[ \chi(x, y) \left( \frac{\partial \chi(x, y)}{\partial y} \right)^2 - \epsilon \frac{\partial^2 \chi(x, y)}{\partial y^2} \right]. \quad (7)$$

The boundary conditions for  $\chi(x, y)$  on  $\Gamma$  and  $\Gamma_C$  are

$$\chi(x, y_\Gamma(x)) = 0, \quad \chi(x, y_C(x)) = 0,$$

respectively. Obviously,

$$\chi(x, y) < 0 \quad (8)$$

for  $(x, y) \in D - \{E \leq E_C\}$ , outside a boundary layer.

The function  $\chi(x, y)$  is one of the most important component of  $P(x, y)$ , and can be expanded in a regular asymptotic power series away from  $\Gamma_C$ ,

$$\chi(x, y) = \chi_0(x, y) + \epsilon \chi_1(x, y) + \dots, \quad (9)$$

where  $\chi_0(x, y)$  satisfies the reduced equation (7), corresponding to  $\epsilon = 0$  and (8). According to [7], for small  $\epsilon$ , the asymptotic approximation to  $P(x, y)$  outside a boundary layer near  $\Gamma_C$  is given by

$$P_0(x, y) = \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\chi_0(x, y)/\sqrt{\epsilon}} e^{-z^2/2} dz. \quad (10)$$

To satisfy the second boundary condition (6), the approximation (10) has to be corrected by an additional boundary layer near  $\Gamma_C$ , as done below.

We found that inside the boundary layer (near  $\Gamma$ ),

$$\frac{\partial \ln P(x, y)}{\partial y} = \frac{\partial P(x, y)/\partial y}{P(x, y)} \approx \frac{1}{\sqrt{\epsilon}} \frac{\partial \chi_0(x, y)}{\partial y} = \sqrt{\frac{1}{\epsilon}} \gamma(x) \frac{\partial \rho(x, y)}{\partial y} + O\left(\frac{\rho}{\sqrt{\epsilon}}\right), \quad (11)$$

where the function  $\gamma(x)$  is a solution of the Bernoulli equation (see [1]) and  $\rho = \rho(x, y)$  is the signed distance from the point  $(x, y)$  to  $\Gamma$ , such that  $\rho < 0$  in  $D$ . Using (11), we can write inside the boundary layer

$$b_2^*(x, y) \approx -\beta y - U'(x) + \sqrt{\epsilon} \beta \gamma(x) \frac{\partial \rho(x, y)}{\partial y}. \quad (12)$$

The asymptotic expansion of  $\partial \ln P(x, y)/\partial y$  near  $\Gamma_C$  was also constructed in the form

$$\frac{\partial \ln P}{\partial y} \approx \frac{y}{\epsilon} \frac{e^\zeta}{e^\zeta - 1}. \quad (13)$$

Here

$$\zeta = \frac{E - E_C}{\epsilon}$$

is the stretched variable,  $E$  is the energy, and  $E_C$  the critical energy measured from the bottom of the well, that is, the height of the barrier. In dimensionless units  $E_C = 1$ .

Then the analysis of the function  $\chi_0(x, y)$  inside a boundary layer near  $\Gamma$ , and then in  $D - \{E \leq E_C\}$ , outside the layer was done. We proved that outside the layer,

$$\frac{\partial \ln P(x, y)}{\partial y} \approx -\frac{1}{\epsilon} \chi_0(x, y) \frac{\partial \chi_0(x, y)}{\partial y}. \quad (14)$$

The two expansions, (13) and (14), have to match near  $\Gamma_C$ , outside the boundary layer. Taking the limit  $\zeta \rightarrow \infty$  in (13), we obtained the form of  $\chi_0(x, y)$  near  $y = y_C(x)$  and also the matched uniform expansion of  $\partial \ln P/\partial y$  (see [1], section 3).

### 3 The exit pdf of the tails

Now we construct the exit pdf,  $p_\Gamma(x)$  of trajectories  $(x^*(t), y^*(t))$  that start at a point  $(x_0, y_0)$  in  $D - \{E \leq E_C\}$ . It is the normalized normal component of the probability

flux density of  $p^*(x, y, \epsilon | x_0, y_0)$ , the solution of the stationary Fokker-Plank equation (FPE)

$$\begin{aligned} & -y \frac{\partial p^*}{\partial x} + \frac{\partial}{\partial y} \left[ \left( \beta y + U'(x) - 2\epsilon\beta \frac{\partial \ln P(x, y)}{\partial y} \right) p^* \right] + \epsilon\beta \frac{\partial^2 p^*}{\partial y^2} \\ & = -\delta(x - x_0, y - y_0) \end{aligned} \quad (15)$$

in  $D - \{E \leq E_C\}$  with the absorbing boundary condition [8]

$$p^*(x, y_\Gamma(x), \epsilon | x_0, y_0) = 0.$$

Choosing  $(x_0, y_0)$  on a contour  $\Gamma_{\epsilon\delta}$  close to  $\Gamma_C$ , the exit pdf is obtained by integrating the normal component of the flux of

$$p^*(x, y, \epsilon) = \oint_{\Gamma_{\epsilon\delta}} p^*(x, y, \epsilon | x_0, y_{\Gamma_{\epsilon\delta}}(x_0)) p_C(x_0) dx_0. \quad (16)$$

## 4 The outer solution

We follow the method of [6] for the asymptotic construction of the solution, with the necessary modifications. The asymptotic solution of the FPE (15) is constructed in the form of an outer solution multiplied by a boundary layer function. A solution of the form

$$p^*(x, y, \epsilon | x_0, y_0) = e^{-\psi(x, y)/\epsilon} Q(x, y, \epsilon), \quad (17)$$

is substituted into the FPE (15) and terms of the same orders of magnitude are balanced. At the leading order  $O(\epsilon^{-1})$ , we find that the function  $\psi(x, y)$  is the solution of the eikonal equation

$$y \frac{\partial \psi}{\partial x} - \left( \beta y + U'(x) - 2\epsilon\beta \frac{\partial \ln P(x, y)}{\partial y} \right) \frac{\partial \psi}{\partial y} + \beta \left( \frac{\partial \psi}{\partial y} \right)^2 = 0. \quad (18)$$

The function  $Q(x, y, \epsilon)$  is assumed to have a finite limit,

$$\lim_{\epsilon \rightarrow 0} Q(x, y, \epsilon) = Q(x, y, 0), \quad (19)$$

for all fixed  $(x, y) \in D - \{E \leq E_C\}$ , and  $Q(x, y, \epsilon)$  has a boundary layer structure near  $\Gamma$  (see Section 5 below). The limit function  $Q(x, y, 0)$  does not vanish in  $D - \{E \leq E_C\}$ , so that for any  $(x, y) \in D - \{E \leq E_C\}$  the essential singularity of  $p^*(x, y, \epsilon | x_0, y_0)$  at  $\epsilon = 0$  is contained in the exponential term in eq.(17).

Using eq.(14), we find that outside the boundary layer near  $\Gamma$  the eikonal equation (18) has the form

$$y \frac{\partial \psi}{\partial x} - \left( \beta y + U'(x) + 2\beta \chi_0(x, y) \frac{\partial \chi_0(x, y)}{\partial y} \right) \frac{\partial \psi}{\partial y} + \beta \left( \frac{\partial \psi}{\partial y} \right)^2 = 0. \quad (20)$$

We use the expansion (13) in the outer region to write the eikonal equation for the outer solution (17) evaluated inside the boundary layer as

$$y \frac{\partial \psi}{\partial x} - (\beta y + U'(x) + 2\gamma^2(x) \rho \rho_y) \frac{\partial \psi}{\partial y} + \beta \left( \frac{\partial \psi}{\partial y} \right)^2 = 0. \quad (21)$$

This outer solution has to be matched by the boundary layer solution in the matching region.

We construct a boundary layer solution of the Fokker-Planck equation (15) by extending the outer approximation of the drift coefficient (14) up to the boundary, rather than using the boundary layer approximation eq.(12). This approximation simplifies the calculations. A similar result is obtained if the approximation (14) is used instead.

Near the saddle point, we can approximate the separatrix by the line  $y = -\lambda x$ . Then  $\rho$  is a linear function of  $(x, y)$  and the coefficients of the first order partial derivatives in the eikonal equation (21) become linear functions. Since the saddle point is a stable attractor of noiseless dynamics, the eikonal function  $\psi(x, y)$  is locally a quadratic form in the neighborhood of the saddle point, that is,

$$\psi(x, y) = \frac{1}{2} (ax^2 + 2bxy + cy^2). \quad (22)$$

Substituting  $\psi$  into equation (21) and simplifying, gives

$$a = \frac{\beta + 2\gamma^2}{\beta} (-\omega^2 + 2\gamma^2\lambda), \quad b = 0, \quad c = \frac{\beta + 2\gamma^2}{\beta}. \quad (23)$$

It follows that the partial derivatives of  $\psi(x, y)$  near the saddle point are given by

$$\psi_y(x, y) = cy, \quad \psi_{yy}(x, y) = c.$$

## 5 The boundary layer equation

The equation for  $Q(x, y)$  is obtained by substituting the solution (17) in the Fokker-Planck equation (15) and setting the sum of the pre-exponential terms that are of order 1 equal to 0. Taking into consideration the eikonal equation (18), we obtain near  $\Gamma$  the equation

$$\begin{aligned} & \beta\epsilon Q_{yy} + (-2\beta\psi_y + \beta y + U'(x) + 2\beta\gamma^2(x)\rho\rho_y) Q_y - yQ_x \\ & + (\beta + 2\beta\gamma^2\rho_y^2 + 2\beta\gamma^2\rho\rho_{yy} - \beta\psi_{yy}) Q = 0 \end{aligned} \quad (24)$$

for  $(x, y) \in D - \{E \leq E_C\}$ . The boundary condition is  $Q(x, y_\Gamma(x)) = 0$ . Next we give the uniform asymptotic approximation to  $p^*(x, y)$ . We introduce the following changes of variables. First, we change  $(x, y) \rightarrow (x, \rho)$  and then scale with

$$\rho = \sqrt{\epsilon}\zeta, \quad x = \epsilon\xi. \quad (25)$$

Now, we introduce the variable

$$\mu = \gamma_1(\xi)\zeta,$$

where  $\gamma_1(x)$  is the solution of the Bernoulli equation

$$-y_\Gamma(x)\gamma_1'(x) + [b_0(x) - \beta\psi''(x) + 2\beta\gamma^2(x)\rho_y^2] \gamma_1(x) = \gamma_1^2(x)\beta\rho_y^2$$

with the initial condition

$$\gamma_1(0) = \sqrt{\frac{b_0(0) - \beta c + 2\beta\gamma^2(0)\rho_y^2(0,0)}{\beta\rho_y^2(0,0)}}.$$

Note that the explicit form of  $b_0(x)$  is given in [1] and [3].

The uniform approximation to  $p^*(x, y, \epsilon | x_0, y_0)$ , valid up to the boundary, is given by

$$p_{unif}(x, y, \epsilon | x_0, y_0) = C|x|^2(\sqrt{1+\beta^2}-1)\tilde{S}(x, y) \exp\left\{-\frac{\psi(x, y)}{\epsilon}\right\}, \quad (26)$$

where  $C$  is a normalization constant and

$$\tilde{S}(x, y) = \sqrt{\frac{2}{\pi}} \int_{\mu}^0 e^{-s^2/2} ds.$$

Note that  $\tilde{S}(x, y_{\Gamma}(x)) = 0$  and for all  $(x, y) \in D - \{E \leq E_C\}$ ,

$$\lim_{\epsilon \rightarrow 0} \tilde{S}(x, y) = 1.$$

The approximation (26) is valid for all  $(x_0, y_0) \in \Gamma_C$ , outside the boundary layer near  $\Gamma$  (that is, for  $y_0 = y_C(x_0)$ ). On the portion of  $\Gamma_C$  contained in the boundary layer near  $\Gamma$  the density  $p_C(x_0)$  is small, because  $p_C(x_0)$  vanishes at  $x_0 = x_C$ . Thus, the uniform approximation to  $p^*(x, y, \epsilon)$ , as defined in eq.(16), is to leading order independent of  $x_0$ . That is,  $p_{unif}(x, y, \epsilon)$  is also given by the right hand side of eq.(26).

Note that  $p_{unif}(x, y, \epsilon)$  satisfies both the boundary condition on  $\Gamma$  and the matching condition in the outer region. The pdf per unit arc length of the exit points on  $\Gamma$  is converted to the pdf per unit  $x$  by the following identities

$$\begin{aligned} \tilde{p}_{\Gamma}(s) ds &= \mathcal{N}^{-1} \mathbf{J}(x, y_{\Gamma}(x)) \cdot \boldsymbol{\nu}(x, y_{\Gamma}(x)) ds \\ &= -\mathcal{N}^{-1} \epsilon \beta \frac{\partial p^*(x, y_{\Gamma}(x))}{\partial y} \nu_2(x, y_{\Gamma}(x)) ds \\ &= -\mathcal{N}^{-1} \epsilon \beta \frac{\partial p^*(x, y_{\Gamma}(x))}{\partial y} dx \\ &= p_{\Gamma}(x) dx, \end{aligned} \quad (27)$$

where the normalization constant is  $\mathcal{N} = -\oint_{\Gamma} \epsilon \beta \frac{\partial p^*(x, y_{\Gamma}(x))}{\partial y} dx$ . Thus  $p_{\Gamma}(x)$  is asymmetric about its maximum and vanishes at the saddle point.

Figure 5.1 shows a histogram of the exit points on  $\Gamma$  vs  $x$ , collected from a direct simulation of eq.(2). Simulations were run with initial conditions given near the bottom of the well. The exit distribution is essentially independent of the initial points of the trajectories of (2), because all trajectories converge first to a neighborhood of the attractor at the bottom of the well and only after a long time there they escape to  $\Gamma$ . Figure 5.2 shows two curves: (a) an analytic curve of eq.(27) which is divided by the area value under the curve, and (b) a curve obtained by interpolating the vertices of the histogram shown in Figure 5.1 (using a polynomial of seventh degree), and then dividing it by the area value appearing under the curve. This means that in Figure 5.2 we see two curves after the normalization process, so that the underlying area is 1. The most likely exit point, denoted  $x_M$ , maximizes  $p_{\Gamma}(x)$ . It is determined by the equation  $p'_{\Gamma}(x) = 0$ , which in view of eq. (22) gives, to leading order,

$$x_M = \sqrt{\frac{2\epsilon(\sqrt{1+\beta^2}-1)}{2ac\lambda^2}}.$$

It follows that the most likely exit point is  $C\sqrt{\varepsilon}$  away from the saddle point.

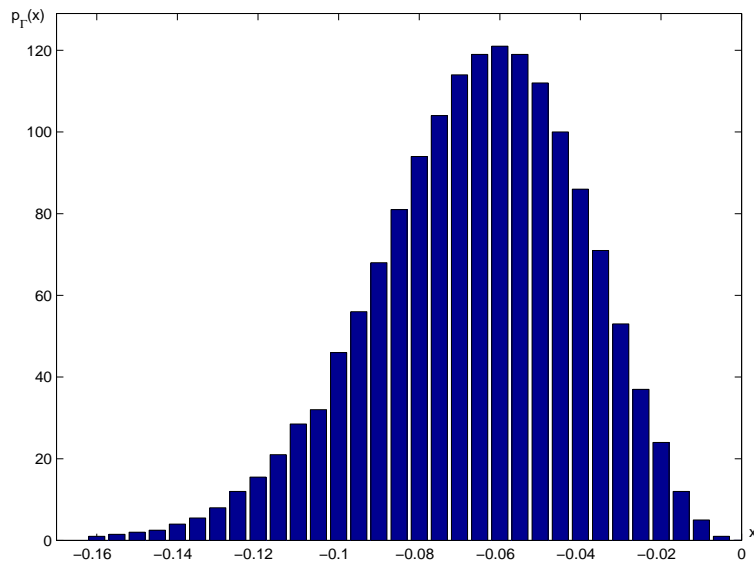


Fig. 5.1. A histogram of the exit points on  $\Gamma$  vs  $x$ . Trajectories of (2) start near the bottom of the well.

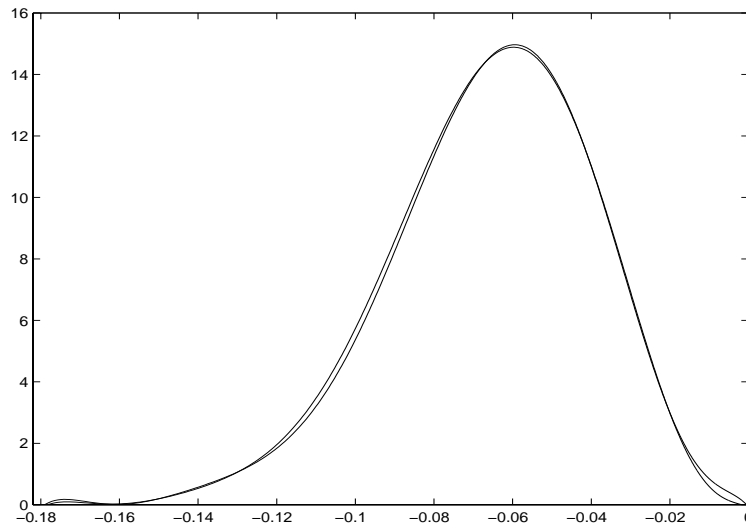


Fig. 5.2. The graphs of the analytic expression eq.(27) and of an interpolated histogram, both normalized so that the underlying area is 1.



## References

- [1] Z. Schuss and A. Spivak, Analytical and Numerical Study of Cramers' Exit Problem I, *Applied Mathematics E-Notes*, 2 (2002), 132–140.
- [2] H. A. Kramers, Brownian motion in a field of force and the diffusion model of chemical reactions, *Physica (Utrecht)*, 7(1940), 284–304.
- [3] B. J. Matkowsky, Z. Schuss and C. Tier, Uniform expansion of the transition rate in Kramers' problem, *J. Stat. Phys.*, 35(3/4)(1984), 443–456.
- [4] M. V. Day, Large Deviation Results for the exit problem with characteristic boundary, *J. Math. Anal. Appl.*, 147(1990), 134–153.
- [5] B. Z. Bobrovsky and O. Zeitouni, *Stochastic Processes and their Applications*, 41(2)(1992), 241–256.
- [6] B. Z. Bobrovsky and Z. Schuss, A singular perturbation method for the computation of the mean first passage time in a nonlinear filter, *SIAM J. Appl. Math.*, 42(1982), 174–187.
- [7] Z. Schuss, *Theory and Applications of Stochastic Differential Equations*, John Wiley and Sons, New York, 1980.
- [8] T. Naeh, M. M. Kłosek, B. J. Matkowsky and Z. Schuss, Direct approach to the exit problem, *SIAM J. Appl. Math.*, 50(1990), 595–627.