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Boundary Behavior of Diffusion Approximations to Markov Jump Processes

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We show that diffusion approximations, including modified diffusion approximations, can be problematic since the proper choice of local boundary conditions (if any exist) is not obvious. For a class of Markov processes in one dimension, we show that to leading order it is proper to use a diffusion (Fokker–Planck) approximation to compute mean exit times with a simple absorbing boundary condition. However, this is only true for the leading term in the asymptotic expansion of the mean exit time. Higher order correction terms do not, in general, satisfy simple absorbing boundary conditions. In addition, the diffusion approximation for the calculation of mean exit times is shown to break down as the initial point approaches the boundary, and leads to an increasing relative error. By introducing a boundary layer, we show how to correct the diffusion approximation to obtain a uniform approximation of the mean exit time. We illustrate these considerations with a number of examples, including a jump process which leads to Kramers' diffusion model. This example represents an extension to a multivariate process.

KEY WORDS: Jump process; master equation; diffusion approximations; boundary conditions; singular perturbations.

1. INTRODUCTION

The problem of approximating a Markov jump process $X(n)$ by a (continuous path) diffusion process $X(t)$ has been the subject of investigation for many years.[(1-5)] For Markov processes that have a single (meta-) stable

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equilibrium state in a given domain D, asymptotic and singular perturbation techniques were recently developed[6–8,11] to construct both the stationary density of fluctuations and the mean escape time from D. Based on these analyses, the question of the validity of diffusion approximations has been clarified. The criterion for the validity depends on the relative size of the first and second conditional moments of the jump process, as described below. However, even when the diffusion approximation appears to be valid, the question of the proper choice of boundary conditions to be used with the diffusion equation for the mean first passage time problem arises.

The mean escape time of the jump process $X(n)$ from D depends on the behavior of $X(n)$ near the boundary ∂D of D. The process $X(n)$ can exit D by jumping over the boundary without hitting it, unlike the continuous diffusion process $X(t)$, which has to hit the boundary to exit D. General asymptotic methods were developed in Refs. 6–8 and 11 for problems where diffusion approximations are not valid. The following question arises in a natural way. Is the mean first passage time of the process $X(n)$ out of D well approximated by that of the approximating diffusion process $X(t)$ when such approximations appear to be valid? The purpose of this paper is to answer this question and to discuss the appropriate boundary conditions (if any) for the approximating diffusions. We show that the mean escape time $\tau(x)$ from D for trajectories of $X(n)$ that start at a point x in D outside a boundary layer near ∂D is well approximated by the escape time of the corresponding diffusion approximation. However, for initial points x in a boundary layer near ∂D, $\tau(x)$ is not well approximated by that of the diffusion approximation and, indeed, the relative error becomes 1 as the initial point approaches ∂D. We show that $\tau(x)$ suffers a discontinuity at ∂D and show how to correct the diffusion approximation to obtain a uniform approximation of $\tau(x)$ whose relative error is uniformly small throughout D. The fact that $\tau(x)$ suffers a discontinuity at ∂D has already been noted in Refs. 11–14 in this context as well as in other problems.

Thus, we consider the process $X(n)$ defined by the stochastic difference equation

$$X(n+1) = X(n) + \varepsilon\xi(n) \tag{1.1}$$

where the conditional jump probability density of the process $\xi(n)$ is given by

$$\begin{aligned}\frac{\partial}{\partial z}\Pr(\xi(n) \leqslant z \mid X(n) = x,\, X(n-1) = x_{n-1}, \ldots, X(0) = x_0)\\ = w(z, x, \varepsilon)\end{aligned} \tag{1.2}$$

with

$$w(z, x, \varepsilon) \sim w_0(z, x) + \varepsilon w_1(z, x) + \cdots \qquad \text{as} \quad \varepsilon \to 0 \tag{1.3}$$

and ε is a small parameter representing, e.g., a measure of jump size relative to system size. The forward Kolmogorov equation (or the master equation) for the transition probability density

$$p(x, y, n, \varepsilon) = \frac{\partial}{\partial y} \Pr(X(n) \leqslant y \mid X(0) = x) \tag{1.4}$$

of the Markov process $X(n)$ is given by[3]

$$p(x, y, n+1, \varepsilon) = \int_{-\infty}^{\infty} p(x, y - \varepsilon z, n, \varepsilon)\, w(z, y - \varepsilon z, \varepsilon)\, dz \tag{1.5}$$

The Kramers–Moyal[1,10] expansion of (1.5) is obtained by expanding the integral in a power series in ε,

$$\begin{aligned} \Delta p &= p(x, y, n+1, \varepsilon) - p(x, y, n, \varepsilon) \\ &= \sum_{n=1}^{\infty} \frac{(-\varepsilon)^n}{n!} \frac{\partial^n}{\partial y^n} \sum_{j=0}^{\infty} \varepsilon^j m_{nj}(y)\, p(x, y, n, \varepsilon) \end{aligned} \tag{1.6}$$

where

$$m_{nj}(y) = \int_{-\infty}^{\infty} z^n w_j(z, y)\, dz \qquad (n = 0, 1, 2,...) \tag{1.7}$$

The mean flow is defined by

$$\dot{x} = m_{11}(x) = \int_{-\infty}^{\infty} z w_1(z, x)\, dz \tag{1.8}$$

where the dot denotes differentiation with respect to the continuous time variable $t = \varepsilon^2 n$. A point x_0 is referred to as an equilibrium in a domain D if it is an equilibrium point of (1.8) in D. As shown in Refs. 6 and 7, the *standard* diffusion approximation obtained by truncating the series in (1.6) at $n = 2$ is valid under the assumption that

$$m_{10}(x) = \int_{-\infty}^{\infty} z w_0(z, x)\, dz = 0 \tag{1.9}$$

Equation (1.6) is then reduced to

$$-\varepsilon^2 \frac{\partial}{\partial y} [m_{11}(y)\, p] + \frac{\varepsilon^2}{2} \frac{\partial^2}{\partial y^2} [m_{20}(y)\, p] + O(\varepsilon^3) = \Delta p \tag{1.10}$$

Expanding

$$p(x, y, n, \varepsilon) \sim p_0(x, y, n) + \varepsilon p_1(x, y, n) + \cdots \tag{1.11}$$

we obtain the Fokker–Planck equation in terms of the continuous time $t = \varepsilon^2 n$ as

$$\frac{\partial p_0}{\partial t} = -\frac{\partial}{\partial y} [m_{11}(y)\, p_0] + \frac{1}{2} \frac{\partial^2}{\partial y^2} [m_{20}(y)\, p_0] \tag{1.12}$$

Equation (1.12) corresponds to the diffusion process $X(t)$ defined by the Itô stochastic differential equation

$$dX = m_{11}(X)\, dt + \sqrt{m_{20}(X)}\, dw(t) \tag{1.13}$$

where $w(t)$ is the standard Brownian motion. We refer to $X(t)$ as the standard diffusion approximation for the jump process $X(n)$, and to Eq. (1.12) as the standard diffusion approximation to (1.5). We observe that the higher order terms in (1.11) are regular perturbations of p_0, so that p_0 is a valid approximation to p on time intervals for which the process $X(n)$ stays in D. This approximation procedure fails if condition (1.9) is not satisfied. Indeed, the Fokker–Planck equation corresponding to a truncation of the series in (1.6) at order ε^2 is given by

$$\frac{\partial \tilde{p}}{\partial t} = -\frac{\partial}{\partial y} \{[m_{10}(y) + \varepsilon m_{11}(y)]\, \tilde{p}\} + \frac{\varepsilon}{2} \frac{\partial^2}{\partial y^2} [m_{20}(y)\, \tilde{p}] \tag{1.14}$$

Equation (1.14) is of singular perturbation type as $\varepsilon \to 0$ $(t = \varepsilon n)$, and in fact

$$\frac{\partial^n}{\partial y^n} \tilde{p} = O\left(\frac{1}{\varepsilon^n}\right) \tilde{p} \tag{1.15}$$

It follows that all terms in the Kramers–Moyal series are $O(1)$ as $\varepsilon \to 0$, and therefore $\tilde{p}$ is not a valid approximation to p. A full discussion of this point was given in Refs. 6 and 7 together with techniques for constructing asymptotic solutions directly from the master equation.

A modified diffusion approximation has been proposed in Ref. 9 with the approximate Fokker–Planck equation

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial y} \{[M_1(y) + \varepsilon M_{11}(y)]\, p\} + \frac{\varepsilon}{2} \frac{\partial^2}{\partial y^2} [M_2(y)\, p] \tag{1.16}$$

The coefficients in (1.16) involve *all* of the moments of the jump process. We refer to Eq. (1.16) as the modified diffusion approximation to (1.5). We describe this procedure in more detail in Section 3.

In Section 2 we discuss the standard diffusion approximation for processes satisfying condition (1.9). In Section 3 we discuss the modified diffusion approximation for processes not satisfying (1.9). In Section 4 we consider some specific examples, including an example of a two-dimensional jump process.

2. BOUNDARY CONDITIONS FOR THE STANDARD DIFFUSION APPROXIMATION

In this section we construct an asymptotic expansion of the mean time for the process $X(n)$ to exit a given domain D. We confine our discussion to processes defined on the real line. We then compare this mean first passage time from D with that of the approximating diffusion process $X(t)$. We now consider the Markov process $X(n)$ defined by (1.1) and (1.2). We assume that the expansion (1.3) is valid and that (1.9) is satisfied in the domain

$$D = \{-\infty < x < B\} \tag{2.1}$$

where $0 < B < \infty$. We assume that all the functions $m_{ij}(x)$ are analytic.

The mean "time" $n(x)$ (the mean number of jumps) to exit D, given $X(0) = x$, is assumed to be finite. Then it is the solution of the equation[6–8,11]

$$\int_{-\infty}^{(B-x)/\varepsilon} n(x + \varepsilon z)\, w(z, x, \varepsilon)\, dz - n(x) = -1 \qquad \text{for} \quad x \in D \tag{2.2}$$

with the boundary condition

$$n(x) = 0 \qquad \text{for} \quad x \geqslant B \tag{2.3}$$

and the condition that $n(x)$ does not grow exponentially as $x \to -\infty$. We construct the outer expansion of the solution $n(x)$ in the form

$$n(x) \sim \frac{n_{-2}(x)}{\varepsilon^2} + \frac{n_{-1}(x)}{\varepsilon} + n_0(x) + \cdots \tag{2.4}$$

as $\varepsilon \to 0$. As shown below, this expansion is valid away from the boundary point $x = B$.

For $B - x \gg \varepsilon$ we perform the following regular perturbation procedure. We substitute (1.3) and (2.4) into (2.2) and extend the upper limit of integration in (2.2) to infinity. We then equate the coefficient of each power of ε separately to zero to obtain a recursive system of equations for the determination of $n_i(x)$. The first two equations are given by

$$L_0 n_{-2}(x) = m_{11}(x) \frac{dn_{-2}(x)}{dx} + \frac{1}{2} m_{20}(x) \frac{d^2 n_{-2}(x)}{dx^2} = -1 \tag{2.5}$$

and

$$L_0 n_{-1}(x) = -m_{12}(x)\frac{dn_{-2}(x)}{dx} - \frac{m_{21}(x)}{2}\frac{d^2 n_{-2}(x)}{dx^2} - \frac{m_{30}(x)}{6}\frac{d^3 n_{-2}(x)}{dx^3} \tag{2.6}$$

Further terms in the expansion can be obtained in a similar manner. We note that Eq. (2.5) is the mean first passage time equation for the approximating diffusion process defined by (1.13).[3–5] To use (2.5) and (2.6) we must prescribe boundary conditions for $n_{-2}(x)$ and $n_{-1}(x)$ at $x = B$. Therefore we next determine these boundary conditions. The continuity of the function $n(x)$ at $x = B$ is not obvious, since cases are known in which $n(x)$ suffers a discontinuity at B.[8,11–16] The fact that $n(B) = 0$ therefore does not necessarily imply that $n(B-) = 0$, and as a matter of fact $n(B-) > 0$ in general. Thus, the values of $n_{-2}(B)$, $n_{-1}(B)$, and so on have to be determined in a consistent way. To complete the analysis a boundary layer expansion is needed. To resolve the question of boundary conditions we will have to match the boundary expansion with the outer expansion. Near the boundary, i.e., for $B - x = O(\varepsilon)$, the upper limit of integration in (2.2) cannot be extended to infinity, so the Kramers–Moyal expansion cannot be employed. We introduce the boundary layer variable

$$\eta = \frac{B - x}{\varepsilon} > 0 \tag{2.7}$$

and the boundary layer function

$$N(\eta) = n(x) \tag{2.8}$$

Since

$$n(x + \varepsilon z) = N(\eta - z) \tag{2.9}$$

eq. (2.22) becomes

$$\int_{-\infty}^{\eta} N(\eta - z)\, w(z, B - \varepsilon\eta, \varepsilon)\, dz - N(\eta) = -1 \qquad \text{for} \quad \eta > 0 \tag{2.10}$$

We assume the expansion

$$N(\eta) \sim \frac{N_{-2}(\eta)}{\varepsilon^2} + \frac{N_{-1}(\eta)}{\varepsilon} + N_0(\eta) + \cdots \tag{2.11}$$

and use the perturbation procedure described above to obtain from (2.10) the following set of equations for $\eta > 0$:

$$\mathscr{L}_0 N_{-2}(\eta) = \int_{-\infty}^{\eta} N_{-2}(\eta - z)\, w_0(z, B)\, dz - N_{-2}(\eta) = 0 \tag{2.12}$$

$$\mathscr{L}_0 N_{-1}(\eta) = \int_{-\infty}^{\eta} \eta N_{-2}(\eta - z)\, w_{0,x}(z, B)\, dz$$
$$- \int_{-\infty}^{\eta} N_{-2}(\eta - z)\, w_1(z, B)\, dz = \mathscr{L}_1 N_{-2}(\eta) \tag{2.13}$$

and

$$\mathscr{L}_0 N_0(\eta) = \mathscr{L}_1 N_{-1}(\eta) - \frac{1}{2}\eta^2 \int_{-\infty}^{\eta} N_{-2}(\eta - z)\, w_{0,xx}(z, B)\, dz$$
$$+ \eta \int_{-\infty}^{\eta} N_{-2}(\eta - z)\, w_{1,x}(z, B)\, dz$$
$$- \int_{-\infty}^{\eta} N_{-2}(\eta - z)\, w_2(z, B)\, dz - 1 \tag{2.14}$$

Here the subscript x denotes partial differentiation with respect to x. From (2.3) we have $N_j(\eta) = 0$ for $\eta \leqslant 0$ and all j. Equation (2.12) is a Wiener–Hopf equation whose solution can be constructed by the Wiener–Hopf method (see, e.g., Ref. 15). The Fourier transform of $N_{-2}(\eta)$ is given by

$$\hat{N}_{-2}(\alpha) = \int_{-\infty}^{\infty} e^{i\alpha\eta} N_{-2}(\eta)\, d\eta = \frac{\Phi(\alpha)}{1 - \hat{w}_0(\alpha, B)} \tag{2.15}$$

where

$$\Phi(\alpha) = \int_{-\infty}^{0} e^{i\alpha\eta} \int_0^{\infty} N_{-2}(z)\, w_0(\eta - z, B)\, dz\, d\eta$$

is an analytic function in the lower half-plane. The function $\Phi(\alpha)$ is defined uniquely up to a multiplicative constant. The function

$$\hat{w}_0(\alpha, B) = \int_{-\infty}^{\infty} e^{i\alpha z} w_0(z, B)\, dz$$

is the characteristic function of the process $\xi(n)$, conditioned on $x = B$.

The matching condition between the outer expansion (2.4) and the boundary layer expansion (2.11) is

$$n(x) - N(\eta) \sim 0$$

as $\varepsilon \to 0$, $x \to B$, and $\eta \to \infty$, to all orders in ε. The behavior of $N_{-2}(\eta)$ as $\eta \to \infty$ is determined by the behavior of $\hat{N}_{-2}(\alpha)$ as $\alpha \to 0$. This in turn is determined by the zero of the denominator in (2.15) at $\alpha = 0$. Since

$$\hat{w}_0(0, B) = \int_{-\infty}^{\infty} w_0(z, B)\, dz = 1 \tag{2.16}$$

and

$$\hat{w}_0'(0, B) = i m_{10}(B) = 0$$

we have

$$1 - \hat{w}_0(\alpha, B) \sim \tfrac{1}{2} m_{20}(B)\, \alpha^2 + \cdots \tag{2.17}$$

and

$$\hat{N}_{-2}(\alpha) = \frac{\Phi(0) + \alpha \Phi'(0) + O(\alpha^2)}{\frac{1}{2}\alpha^2 m_{20}(B) + \frac{i}{6} m_{30}(B)\, \alpha^3 + O(\alpha^4)} = \frac{a_{-2}}{\alpha^2} + \frac{a_{-1}}{\alpha} + \cdots \tag{2.18}$$

where

$$a_{-2} = \frac{2\Phi(0)}{m_{20}(B)}; \qquad a_{-1} = \frac{2\Phi'(0)}{m_{20}(B)} - \frac{2i\Phi(0)\, m_{30}(B)}{3m_{20}^2(B)} \tag{2.19}$$

and so on. Hence,

$$N_{-2}(\eta) = -[(ia_{-1} + a_{-2}\eta) + o(1)] \qquad \text{as} \quad \eta \to \infty \tag{2.20}$$

where $\Phi(0)$ is an as yet undetermined constant, whose value uniquely determines $\Phi(\alpha)$. We determine the constants $\Phi(0)$ and $n_{-2}(B)$ by matching the outer expansion (2.4) as $x \to B$ with the boundary layer expansion (2.11) as $\eta \to \infty$. We obtain to leading order $[O(1/\varepsilon^2)]$

$$n_{-2}(x) - N_{-2}(\eta) = n_{-2}(B) + ia_{-1} + a_{-2}\eta \to 0 \tag{2.21}$$

as $\varepsilon \to 0$ and $\eta \to \infty$. Hence $a_{-2} = 0$ and consequently $\Phi(0) = 0$, so that $\Phi(\alpha) = 0$ and

$$n_{-2}(B) = 0 \tag{2.22}$$

Condition (2.22) shows that $n_{-2}(x)$ is continuous at the boundary $x = B$.

Next we calculate $n_{-1}(B)$. To this end we solve Eq. (2.13) for $N_{-1}(\eta)$. Since $N_{-2}(\eta) = 0$ by (2.20) and (2.22), Eq. (2.13) is again a Wiener–Hopf equation with solution (2.15), and thus

$$N_{-1}(\eta) = -[(ia_{-1} + \eta a_{-2}) + o(1)] \qquad \text{as} \quad \eta \to \infty \tag{2.23}$$

where $\Phi(0)$ is again an undetermined constant. Using

$$\frac{n_{-2}(x)}{\varepsilon^2} = -\frac{n'_{-2}(B)(B-x)+\cdots}{\varepsilon^2} = -\frac{n'_{-2}(B)\,\eta}{\varepsilon}+\cdots \tag{2.24}$$

which follows from (2.22), the matching condition at order $O(1/\varepsilon)$ is given by

$$n_{-1}(B)-n'_{-2}(B)\,\eta-N_{-1}(\eta)\to 0 \qquad \text{as} \quad \eta\to\infty \tag{2.25}$$

With (2.23) the condition (2.25) gives

$$-ia_{-1}=n_{-1}(B); \qquad a_{-2}=n'_{-2}(B)$$

and hence

$$n_{-1}(B)=-\frac{ia_{-1}}{a_{-2}}n'_{-2}(B) \tag{2.26}$$

It follows that $n(x)$ suffers a discontinuity at $x=B$, since $n(x)=0$ for $x\geqslant B$. The discontinuity in $n(x)$ is of order $1/\varepsilon$, or more specifically

$$n(B-)-n(B+)=\frac{N_{-1}(0)}{\varepsilon}+O(1) \qquad \text{as} \quad \varepsilon\to 0 \tag{2.27}$$

The mean number of jumps to leave D predicted by the diffusion approximation (1.13) is given by

$$n_d(x)=n_{-2}(x)/\varepsilon^2 \tag{2.28}$$

Hence the relative error in using the diffusion approximation, given by

$$e_d(x)=[n(x)-n_d(x)]/n(x) \tag{2.29}$$

satisfies

$$e_d(x)\to 0 \quad \text{as} \quad \varepsilon\to 0 \qquad \text{for} \quad B-x\gg\varepsilon \tag{2.30}$$

However, this is not the case near $x=B$, since

$$e_d(B)\to 1 \qquad \text{as} \quad \varepsilon\to 0 \tag{2.31}$$

Therefore the diffusion approximation with absorbing conditions at B correctly predicts the mean first passage time for initial conditions outside the boundary layer at $x=B$, i.e., for $B-x\gg\varepsilon$. For initial conditions approaching the boundary the diffusion approximation leads to increasingly large errors.

A better approximation is obtained if $n_d(x)$ is replaced by the uniform expansion

$$n_{db}(x)=\frac{n_{-2}(x)}{\varepsilon^2}+\frac{n_{-1}(x)}{\varepsilon}+\frac{N_{-1}[(B-x)/\varepsilon]-n_{-1}(B)-n'_{-2}(B)(x-B)/\varepsilon}{\varepsilon} \tag{2.32}$$

For $n_{db}(x)$ the relative error satisfies

$$e_{db}(x)=O(\varepsilon) \qquad \text{for all} \quad x\in D \tag{2.33}$$

We observe that the escape rate from D does not increase to infinity as $x\to B$, but rather becomes $O(1/\varepsilon)$.

We turn now to the analysis of continuous-time Markov jump processes. Let $X(t)$ be a Markov process defined by continuous dynamics between jumps and assume the jumps occur at exponential waiting times. Thus

$$\begin{gathered} X(t+\Delta t)=X(t)+b(x,\varepsilon)\,\Delta t+o(\Delta t)\\ \text{w.p. } 1-\frac{\lambda(x)}{\varepsilon}\Delta t+o(\Delta t) \end{gathered} \tag{2.34}$$

and

$$\begin{gathered} X(t+\Delta t)=X(t)+b(x,\varepsilon)\,\Delta t+\varepsilon\xi(t)+o(\Delta t)\\ \text{w.p. } \frac{\lambda(x)}{\varepsilon}\Delta t+o(\Delta t) \quad \text{as} \quad \Delta t\to 0 \end{gathered} \tag{2.35}$$

The conditional probability density of $\xi(t)$ is given by

$$\begin{aligned} &\frac{\partial}{\partial z}\Pr(\xi(t)\leqslant z\mid X(t)=x,\, X(t_{n-1})=x_{n-1},\dots,\, X(0)=x_0)\\ &\quad =w(z,x,\varepsilon) \end{aligned} \tag{2.36}$$

for all $t>t_{n-1}>\cdots>t_0$ and all $x, x_{n-1},\dots, x_0$. Equations (2.34)–(2.36) define $X(t)$ as a continuous-time Markov process. The forward Kolmogorov equation for the transition probability density of $X(t)$ is given by

$$\begin{aligned} \frac{\partial p}{\partial t}= &-\frac{\partial}{\partial y}[b(y,\varepsilon)\,p]\\ &+\frac{1}{\varepsilon}\int_{-\infty}^{\infty}\lambda(y-\varepsilon z)\,p(x,y-\varepsilon z,t)\,w(z,y-\varepsilon z,\varepsilon)\,dz\\ &-\frac{\lambda(y)}{\varepsilon}\,p(x,y,t) \end{aligned} \tag{2.37}$$

We assume

$$b(y, \varepsilon) \sim b_0(y) + \varepsilon b_1(y) + \cdots \tag{2.38}$$

and that $w(z, x, \varepsilon)$ has the expansion (1.3) as $\varepsilon \to 0$. The analysis of (2.37) is analogous to that of (1.5). The conditional moments $m_{nj}(x)$ in (1.6) are now replaced by

$$\begin{aligned} \tilde{m}_{1j}(x) &= b_j(x) + \lambda(x)\, m_{1j}(x) \\ \tilde{m}_{nj}(x) &= \lambda(x)\, m_{nj}(x), \qquad n > 1 \end{aligned} \tag{2.39}$$

Thus the standard diffusion approximation is valid if we assume that

$$\tilde{m}_{10}(x) = 0 \tag{2.40}$$

The mean first passage time $\tau(x)$ for the process $X(t)$ to exit D, given the initial condition $X(0) = x$, satisfies

$$\begin{aligned} b(x, \varepsilon)\, \tau'(x) + \frac{\lambda(x)}{\varepsilon} \int_{-\infty}^{(B-x)/\varepsilon} \tau(x + \varepsilon z)\, w(z, x, \varepsilon)\, dz \\ - \frac{\lambda(x)}{\varepsilon} \tau(x) = -1 \qquad \text{for} \quad x < B \end{aligned} \tag{2.41}$$

and

$$\tau(x) = 0 \qquad \text{for} \quad x \geqslant B \tag{2.42}$$

When $B - x \gg \varepsilon$ we seek an asymptotic solution of (2.4) in the form

$$\tau(x) = \tau_{-1}(x)/\varepsilon + \tau_0(x) + \cdots \tag{2.43}$$

Following the perturbation procedure described above, we obtain to leading order

$$\tilde{L}_0 \tau_{-1}(x) = \tfrac{1}{2} \tilde{m}_{20}(x)\, \tau''_{-1}(x) + \tilde{m}_{11}(x)\, \tau'_{-1}(x) = -1, \qquad x < B \tag{2.44}$$

with $\tau_{-1}(B) = 0$, and to the next order

$$\tilde{L}_0 \tau_0(x) = -\tilde{m}_{12}(x)\, \tau'_{-1}(x) - \frac{1}{2} \tilde{m}_{21}(x)\, \tau''_{-1}(x) - \frac{1}{6} \tilde{m}_{30}(x)\, \tau'''_{-1}(x) \tag{2.45}$$

with

$$\tau_{-1}(B) = -(i\tilde{a}_{-1}/\tilde{a}_{-2})\, \tau'_{-1}(B)$$

Here $\tilde{a}_{-j}$ $(j=1, 2)$ are determined by (2.19) with m_{j0} replaced by $\tilde{m}_{j0}$ $(j=1, 2, 3)$, and

$$\tilde{m}_{20}(x)=\lambda(x)\, m_{20}(x) \tag{2.46}$$

The conclusion is therefore the same as in (2.27)–(2.33).

3. THE MODIFIED DIFFUSION APPROXIMATION

When (1.9) is not satisfied, the standard diffusion approximation to the process $X(n)$ [cf. (1.1)] is valid only for the description of relatively small fluctuations about a (meta-) stable equilibrium point, say at $x=0$. For this case a modified Fokker–Planck equation of the form (1.16) has been proposed in Ref. 9. We give here an alternative derivation of (1.16), based on Refs. 6–8 and 11. It has been shown in Refs. 8 and 11 that the (quasi) steady-state probability density function of the process $X(n)$ in D is given asymptotically by

$$p(x) \sim e^{-\psi(x)/\varepsilon} \sum_{i=0}^{\infty} K_i(x)\, \varepsilon^i \tag{3.1}$$

Here $\psi'(x)$ is the nonzero solution of the equation

$$\int_{-\infty}^{\infty} e^{z\psi'(x)} w_0(z, x)\, dz = 1 \tag{3.2}$$

Equation (3.2) can be written as the equation (for t)

$$\Phi_0(t, x)=1 \tag{3.3}$$

where $\Phi_0(t, x)$ is the first term in the expansion of the stationary conditional moment generating function $\Phi(t, x)$ of the process $\xi(n)$,

$$E(e^{t\xi(n)} \mid X(n)=x)=\Phi(t, x) \sim \Phi_0(t, x)+\varepsilon\Phi_1(t, x)+\cdots \tag{3.4}$$

The function $K_0(x)$ is given by

$$K_0(x)=K_{01}(x)\, K_{02}(x) \tag{3.5}$$

with

$$K_{01}(x)=\exp\left(-\int_0^x \frac{I_2(y)}{2I_1(y)}\, dy\right) \Big/ \sqrt{I_1(x)} \tag{3.6}$$

where

$$I_1(x)=\frac{\partial}{\partial t}\, \Phi_0(t, x)\Big|_{t=\psi'(x)} \tag{3.7}$$

and

$$I_2(x) = \frac{\partial^2}{\partial t\, \partial x} \Phi_0(t, x)\bigg|_{t=\psi'(x)} \tag{3.8}$$

The function $K_{02}(x)$ is given by

$$K_{02}(x) = \exp\left[\int_0^x \frac{\Phi_1(\psi'(y), y)}{I_1(y)}\, dy\right] \tag{3.9}$$

We wish to determine the coefficients M_1, M_{11}, and M_2 in (1.16), by requiring the solution of (1.16) to agree with the leading term of the expansion (3.1) of the solution of the master equation (1.5). This requirement determines two relations between the three coefficients in terms of ψ and K_0. These relations are

$$2M_1(x)/M_2(x) = -\psi'(x) \tag{3.10}$$

and

$$\left[\exp \int_0^x \frac{2M_{11}(t)}{M_2(t)}\, dt\right] \Big/ M_2(x) = K_0(x) \tag{3.11}$$

where $\psi'(x)$ is defined by (3.2) and $K_0(x)$ by (3.5). We note that the formula for $M_2(x)$ in Ref. 9 can be obtained by expanding $e^{z\psi'}$ in (3.2), solving for $m_{10}(x)/\psi'(x)$, and using the result in (3.10). A third condition is necessary to determine the coefficients uniquely. This condition may be chosen in various ways. In Ref. 9, $M_1(x)$ is chosen to be $m_{10}(x)$, so as to preserve the limiting drift equation $\dot{x} = M_1(x) = m_{10}(x)$. We observe that other choices are clearly possible. Indeed, since for long time, drift equations are relevant only near equilibrium points, only the linear part of $m_1(x)$ near an equilibrium point is important. Thus, any choice that satisfies (3.10) and (3.11) and has the correct behavior near equilibrium points would appear to be equally good.

If B is a *characteristic* boundary point, i.e., if

$$m_1(x) \sim \sum_{j=0}^{\infty} m_{1j}(x)\, \varepsilon^j$$

satisfies

$$m_1(B) = 0, \qquad m_1(x) < 0 \qquad \text{for} \quad 0 < x < B \tag{3.12}$$

and

$$m_1(x) > 0 \qquad \text{for} \quad x > B$$

then the expected first passage time from the equilibrium point at 0 to B for the modified diffusion approximation (1.16), with $M_2(x)$ and $M_{11}(x)$ defined by (3.10) and (3.11), respectively, agrees to leading order with that of the process $X(n)$. The asymptotic expression for the expected time for the process $X(n)$ to exit D, given $X(0)=0$, is given by[8,11]

$$n(0) \sim \frac{\pi}{\varepsilon} \frac{K_0(0)}{K_0(B)} e^{\psi(B)/\varepsilon} \left| \frac{m_{20}(0)}{m'_{10}(0)} \frac{m_{20}(B)}{m'_{10}(B)} \right|^{1/2} \frac{1}{m_{20}(B)} \tag{3.13}$$

If, however, the initial point $X(0)=x$ is in an ε neighborhood of B, the mean time predicted by the modified diffusion approximation (1.16) is inaccurate. The uniform expansion of $n(x)$ was given in Refs. 8 and 11 as

$$n(x) \sim n(0) \begin{cases} 2\left(\dfrac{m'_{10}(B)}{\pi m_{20}(B)}\right)^{1/2} \displaystyle\int_0^{(B-x)/\sqrt{\varepsilon}} \exp\left(-\dfrac{m'_{10}(B)\, u^2}{m_{20}(B)}\right) du & \text{for } B-x \gg \varepsilon \\ U_0\left(\dfrac{B-x}{\varepsilon}\right)\sqrt{\varepsilon} & \text{for } B-x=O(\varepsilon) \end{cases} \tag{3.14}$$

where $U_0(\eta)$ is the solution of the Wiener–Hopf equation

$$\mathscr{L}_0 U_0(\eta)=0 \tag{3.15}$$

with $\mathscr{L}_0$ defined in (2.12), and the matching condition

$$U_0(\eta) \sim 2\left(\frac{m'_{10}(B)}{\pi m_{20}(B)}\right)^{1/2} \eta \qquad \text{for } \eta \gg 1 \tag{3.16}$$

When B is a noncharacteristic boundary, i.e.,

$$m_{10}(B)<0 \tag{3.17}$$

the modified diffusion approximation (1.16) with an absorbing boundary condition at $x=B$ is not a good approximation to $X(n)$. As a matter of fact, no simple (local) boundary conditions to be used with the modified diffusion approximation (1.16), that lead to an accurate approximation of the mean exit time, are known. The uniform expansion of $n(x)$ for a noncharacteristic boundary is given by

$$n(x)=n(0)\, U_0\left(\frac{B-x}{\varepsilon}\right) \tag{3.18}$$

with

$$n(0) \sim \left(\frac{2\pi}{\psi''(0)\,\varepsilon}\right)^{1/2} \frac{K_0(0)}{K_0(B)} \times \frac{\exp[\psi(B)/\varepsilon]}{\int_{-\infty}^{0} e^{\eta\psi'(B)} \int_{-\infty}^{\eta} w_0(z, B)\, U_0(\eta - z)\, dz\, d\eta} \tag{3.19}$$

(see Refs. 8 and 11). Here $U_0(\eta)$ is the solution of (3.15) with the matching condition

$$U_0(\eta) \to 1 \qquad \text{as} \quad \eta \to \infty$$

In contrast to approaches based on diffusion approximations, either standard or modified, both of which require the addition of local boundary conditions, the methods developed in Refs. 6–8 and 11 give a general approach to the solution of equations (1.1) or (2.44) (2.45). These methods lead to explicit asymptotic expansions for the stationary probabilities and mean first passage times and do not require replacing the original boundary conditions (if any) by local boundary conditions. In addition, these methods lead to a systematic approach to obtaining corrections to the leading term.

4. APPLICATIONS AND EXAMPLES

We now present two examples which illustrate how to incorporate boundary corrections into diffusion approximations. Thus, we first consider a jump process on the lattice $\{n\varepsilon \mid n = 0, \pm 1, \pm 2,...\}$ which jumps one step to the left with probability $l(x, \varepsilon)$ and either one or two steps to the right with probability $r_1(x, \varepsilon)$ or $r_2(x, \varepsilon)$, respectively (see Fig. 1). An example of a symmetric $(l_1 = r_1, l_2 = r_2)$ two-step random walk was considered in Ref. 16, where the jump probabilities were assumed constant. Thus the

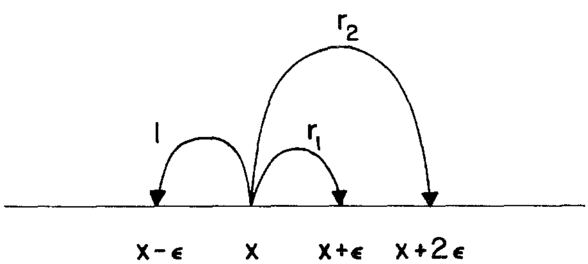

Fig. 1. Sketch of possible jumps from the point x, with the probabilities of each jump indicated.

process had zero drift and the master equation could be explicitly solved. In contrast, our process is nonsymmetric with nonconstant jump probabilities. Other examples of random walks and their approximations are discussed in the review article by Weiss and Rubin.[17]

Thus

$$\begin{aligned} w(z, x, \varepsilon) = l(x, \varepsilon)\, \delta(z+1) + [1 - l(x, \varepsilon) - r_1(x, \varepsilon) - r_2(x, \varepsilon)]\, \delta(z) \\ + \delta(z-1)\, r_1(x, \varepsilon) + \delta(z-2)\, r_2(x, \varepsilon) \end{aligned} \tag{4.1}$$

We assume that first moment $m_1(x, \varepsilon)$ is $O(\varepsilon)$, i.e.,

$$m_1(x, \varepsilon) = -l(x, \varepsilon) + r_1(x, \varepsilon) + 2r_2(x, \varepsilon) = \varepsilon m_{11}(x) \tag{4.2}$$

so that (1.9) is satisfied. It follows that the second and third moments are given by

$$\begin{aligned} m_2(x, \varepsilon) &= 2r_1(x, \varepsilon) + 6r_2(x, \varepsilon) - \varepsilon m_{11}(x) = m_{20}(x) + \varepsilon m_{21}(x) \\ m_3(x) &= 6r_2(x, \varepsilon) + \varepsilon m_{11}(x) = m_{30}(x) + \varepsilon m_{31}(x) \end{aligned} \tag{4.3}$$

Setting $t = \varepsilon^2 n$ and treating x and t as continuous variables, we obtain the standard diffusion approximation for this process as given by the Itô equation

$$dx = m_{11}(x)\, dt + \sqrt{m_{20}\,(x)}\, dw \tag{4.4}$$

The Fokker–Planck equation for (4.4) is

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}\,[m_{11}(x)\, p] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\,[m_{20}(x)\, p] = Lp \tag{4.5}$$

The mean number of jumps $n(x)$ to exit D, given $X(0) = x$, is given by

$$n_B(x) \sim \frac{n_{-2}(x)}{\varepsilon^2} + \frac{n_{-1}(x)}{\varepsilon} + \cdots \tag{4.6}$$

where

$$L^* n_{-2}(x) = m_{11}(x)\frac{dn_{-2}(x)}{dx} + \frac{m_{20}(x)}{2}\frac{d^2 n_{-2}(x)}{dx^2} = -1 \quad \text{for } x < B \tag{4.7}$$

with the boundary condition

$$n_{-2}(B) = 0$$

and the condition that $n_{-2}(x)$ does not grow exponentially as $x \to -\infty$. The correction $n_{-1}(x)$ is the solution of

$$L^* n_{-1}(x) = -\frac{1}{2} m_{21}(x) \frac{d^2 n_{-2}(x)}{dx^2} - \frac{m_{30}(x)}{6} \frac{d^3 n_{-2}(x)}{dx^3} \quad \text{for } x < B \tag{4.8}$$

with

$$n_{-1}(B) = A n'_{-2}(B)$$

and the growth condition as $x \to -\infty$ imposed on $n_{-2}(x)$. Equation (2.26) implies that the constant A is given by

$$A = -\frac{[r_1(B,0) + 2r_2(B,0)]\, r_2(B,0)}{[r_1(B,0) + 3r_2(B,0)][3r_1(B,0) + 4r_2(B,0)]} \tag{4.9}$$

The function $N_{-1}(\eta)$ is given by

$$N_{-1}(\eta) = -n'_{-2}(B) \left\{ \eta - \frac{l(B,0)\, r_2(B,0)}{[l(B,0) + r_2(B,0)][r_1(B,0) + 2l(B,0)]} \times \left[1 - \left(\frac{-r_2(B,0)}{l(B,0)} \right)^{\eta} \right] \right\} \tag{4.10}$$

Hence

$$\begin{aligned} n_{db}(x) &= \frac{n_{-2}(x)}{\varepsilon^2} + \frac{n_{-1}(x)}{\varepsilon} \\ &\quad - \frac{n'_{-2}(B)}{\varepsilon} \frac{l(B,0)\, r_2(B,0)}{[l(B,0) + r_2(B,0)][r_1(B,0) + 2l(B,0)]} \\ &\quad \times \left(\frac{-r_2(B,0)}{l(B,0)} \right)^{(B-x)/\varepsilon} \end{aligned} \tag{4.11}$$

Thus, e.g., the mean number of steps required to reach or exceed B, starting one lattice point away from B, is given by

$$\begin{aligned} n(B-\varepsilon) &\approx n_{db}(B-\varepsilon) \\ &= -\frac{n'_{-2}(B)}{\varepsilon} \frac{r_1(B,0) + l(B,0) - r_2(B,0)}{r_1(B,0) + 2l(B,0)} [1 + o(1)] \end{aligned}$$

Thus, if absorbing boundary conditions are employed with the diffusion approximation, the absolute error in the mean exit time will be $O(1/\varepsilon)$, and the relative error will be $O(\varepsilon)$ if x is bounded away from $x = B$, but will be $O(1)$ if x is within $O(\varepsilon)$ of the boundary point $x = B$. In contrast, for the correct boundary condition, the relative error is uniformly $O(\varepsilon)$ throughout the domain.

Next we give an application to Kramers' diffusion problem. We consider a particle of mass M whose motion between collisions with small particles of mass m (with $m \ll M$) is governed by the equations

$$\dot{X} = Y, \qquad \dot{Y} = -U'(X) \tag{4.12}$$

where $U(x)$ is the potential whose graph is shown in Fig. 2. The small particles have velocity $\pm(kT/m)^{1/2}$ with probability 1/2, where k is Boltzmann's constant and T is temperature. Consequently, if ξ is the random velocity of the small particles, then

$$\langle \xi \rangle = 0, \qquad \langle \xi^2 \rangle = kT/m \tag{4.13}$$

This distribution, which matches the first two moments of the Maxwell–Boltzmann distribution, is chosen for its simplicity. Upon collision, the value of the velocity Y changes according to the law of an elastic collision. Thus, the motion of the particle in phase space is a stochastic process $(X(t), Y(t))$. If ΔY is the change in velocity, given a velocity Y of the heavy particle,

$$\Delta Y = (\xi - Y)\frac{2m}{M + m} \tag{4.14}$$

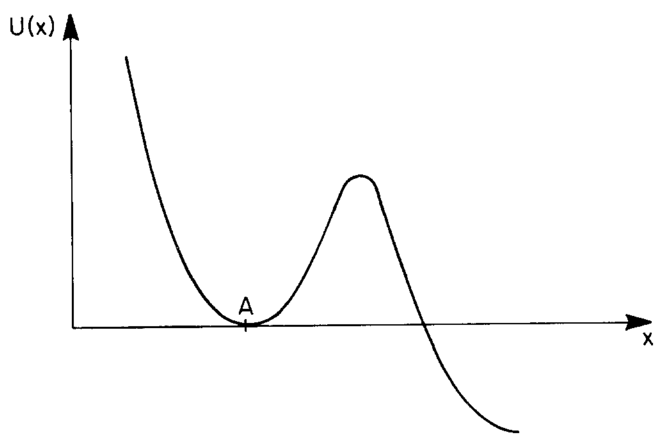

Fig. 2. Sketch of the potential $U(x)$.

Here $2m/(M+m) \approx 2m/M$ is the reduced mass for the collision. The probability density for the time between collisions follows an exponential distribution with parameter $\alpha = M\beta/m$, so that β is a measure of "viscosity." In order to use this model to calculate the escape rate of the heavy particle from the potential well we denote by D the domain of attraction in phase space of the stable equilibrium point $x = A$, $y = 0$, and by Γ its boundary (the "separatrix" defined below). The escape rate is inversely proportional to the mean time τ to cross Γ. The mean time $\tau(x, y)$, conditioned on the initial values $X(0) = x$, $Y(0) = y$, is the solution of the equation[6]

$$L\tau = y\frac{\partial \tau}{\partial x} - U'(x)\frac{\partial \tau}{\partial y} + \frac{M\beta}{4m}\left\{\tau\left(x,\, y + \frac{2m}{M}\left[\left(\frac{kT}{m}\right)^{1/2} - y\right]\right)\right.$$
$$\left. + \tau\left(x,\, y + \frac{2m}{M}\left[-\left(\frac{kT}{m}\right)^{1/2} - y\right]\right) - 2\tau(x, y)\right\} = -1 \quad \text{for } (x, y) \in D \tag{4.15}$$

and

$$\tau(x, y) = 0 \qquad \text{for} \quad (x, y) \notin D$$

Setting $\varepsilon^2 = m/M$, we find for (4.14) the form

$$L\tau = y\tau_x - U'(x)\,\tau_y + \frac{\beta}{4\varepsilon^2}\left[\tau\left(x,\, y - 2\varepsilon^2 y + 2\varepsilon\left(\frac{kT}{M}\right)^{1/2}\right)\right.$$
$$\left. + \tau\left(x,\, y - 2\varepsilon^2 y - 2\varepsilon\left(\frac{kT}{M}\right)^{1/2}\right) - 2\tau(x, y)\right] = -1 \tag{4.16}$$

This model was proposed in Ref. 18, where weak convergence of the jump process $(X(t), Y(t))$ to a diffusion process as $\varepsilon \to 0$ was shown for time intervals of order $1/\varepsilon$. In Ref. 6 we showed that the standard diffusion approximation was valid and that it was described by Kramers' backward equation

$$\frac{\partial p}{\partial t} = L_0 p = y p_x - [U'(x) + \beta y]\, p_y + \frac{\beta k T}{M} p_{yy} \tag{4.17}$$

where p is the density in phase space. Equation (4.17) is the backward Kolmogorov equation corresponding to the diffusion approximation defined by the stochastic system

$$\dot{x} = y, \qquad \dot{y} = -U'(x) - \beta y + (2\beta kT/M)^{1/2}\,\dot{w} \tag{4.18}$$

where $w(t)$ is a Brownian motion. We define the domain D as the domain of attraction of the stable equilibrium state of (4.18) with $T = 0$, and Γ as its boundary. The mean time τ_0 for the diffusion approximation to $(X(t), Y(t))$ to hit Γ is the solution of

$$L_0\tau_0 = -1 \qquad \text{in } D \tag{4.19}$$

$$\tau_0 = 0 \qquad \text{on } \Gamma \tag{4.20}$$

We now show that this approximation is valid for initial conditions inside D, outside a boundary layer near Γ. Near Γ a correction is needed, as in the previous example. In addition, τ suffers a jump discontinuity of order ε at Γ. Thus, expanding

$$\tau = \tau_0 + \varepsilon\tau_1 + \cdots \tag{4.21}$$

we find that τ_0 satisfies (4.19), and

$$L_0\tau_1 = L_1\tau_0 = 0 \tag{4.22}$$

and so on. To determine the boundary conditions we consider Eq. (4.16) in the boundary layer. We scale near any boundary point (x, y_0) by

$$\eta = (y_0 - y)/\varepsilon, \qquad \eta > 0 \tag{4.23}$$

and define

$$\tau(x, y) = T(x, \eta) \tag{4.24}$$

Equation (4.16) is then

$$(y_0 - \varepsilon\eta)\, T_x + \frac{U'(x)}{\varepsilon} T_\eta + \frac{\beta}{4\varepsilon^2}\left\{T\left(x, \eta - 2\left(\frac{kT}{M}\right)^{1/2} + 2\varepsilon(y_0 - \varepsilon\eta)\right)\right.$$
$$\left. +\; T\left(x, \eta + 2\left(\frac{kT}{M}\right)^{1/2} + 2\varepsilon(y_0 - \varepsilon\eta)\right) - 2T(x, \eta)\right\} = -1 \tag{4.25}$$

for $\eta > 0$, and

$$T(x, \eta) = 0 \qquad \text{for} \quad \eta \leqslant 0 \tag{4.26}$$

We expand

$$T \sim T_0 + \varepsilon T_1 + \cdots \tag{4.27}$$

and obtain to leading order $O(1/\varepsilon^2)$

$$\mathscr{L}_0 T_0 = T_0\left(x, \eta - 2\left(\frac{kT}{M}\right)^{1/2}\right) + T_0\left(x, \eta + 2\left(\frac{kT}{M}\right)^{1/2}\right) - 2T_0(x, \eta) = 0$$
$$\text{for} \quad \eta > 2\left(\frac{kT}{M}\right)^{1/2} \tag{4.28}$$

and

$$T_0\left(x, \eta + 2\left(\frac{kT}{M}\right)^{1/2}\right) = 2T_0(x, \eta) \qquad \text{for} \quad 0 < \eta \leqslant 2\left(\frac{kT}{M}\right)^{1/2} \tag{4.29}$$

Hence, on the lattice $\eta = 2(kT/M)^{1/2}\, n$, $n = 1, 2, \ldots$,

$$T_0\left(x, 2\left(\frac{kT}{M}\right)^{1/2} n+\right) = T_0(x, 0+)(1+n) \tag{4.30}$$

where $T_0(x, 0+)$ is an undetermined function. Matching the expansion (4.27) with (4.21) as $y \to y_0$, $\varepsilon \to 0$, and $\eta \to \infty$ through the lattice points, we obtain

$$T_0(x, 0+) = 0 \tag{4.31}$$

so that

$$T_0(x, \eta) = 0 \tag{4.32}$$

and consequently

$$\tau_0(x, y_0) = 0 \tag{4.33}$$

At the next order, we obtain

$$\mathscr{L}_0 T_1 = 0 \tag{4.34}$$

since $T_0 = 0$. Using (4.30) and (4.31) in the equations for T_1, we obtain

$$T_1\left(x, 2\left(\frac{kT}{M}\right)^{1/2} n+\right) = T_1(x, 0+)(1+n), \qquad n = 0, 1, \ldots \tag{4.35}$$

where $T_1(x, 0+)$ is to be determined by matching. Proceeding as above, we obtain

$$\tau_1(x, y) - \eta\tau_{0,y}(x, y) - T_1(x, \eta) \to 0 \tag{4.36}$$

as $y \to y_0$ and $\varepsilon \to 0$ on the lattice. It follows that

$$\tau_{0,y}(x, y_0) = -T_1(x, 0+) \tag{4.37}$$

and

$$\tau_1(x, y_0) = T_1(x, 0+)\, 2(kT/M)^{1/2}$$

Thus

$$\tau_1(x, y_0) = -2(kT/M)^{1/2}\,\tau_{0,y}(x, y_0) \tag{4.38}$$

It follows that $\tau(x, y)$ suffers a discontinuity of size

$$\varepsilon T_1(x, 0+) = -(m/M)^{1/2}\,\tau_{0,y}(x, y_0)$$

at Γ. At boundary points (x, y_0) where $\tau_{0,y}(x, y_0) = 0$, the discontinuity is of order ε^2.

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