PRINCIPAL EIGENVALUE CHARACTERIZATION CONNECTED WITH STOCHASTIC PARTICLE MOTION IN A FINITE INTERVAL¹

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In this paper, we show that despite their distinction, both the Statonovich and $\hat{\text{Ito}}$ calculi lead to the same reactive Fokker-Planck equation:

$$\frac{\partial p}{\partial t} - \frac{\partial}{\partial x} \left[D \frac{\partial p}{\partial x} - bp \right] = \lambda m p, \quad (1)$$

describing stochastic dynamics of a particle moving under the influence of an indefinite potential $m(x, t)$, a drift $b(x, t)$, and a constant diffusion D . We treat the periodic-parabolic eigenvalue problem (1) for finite domains having absorbing barriers. We show that under conditions required by the maximum principle, the positive principal eigenvalue λ^* (and the negative principal eigenvalue λ_*) is connected to the probability eigendensity function $p(x, t)$ by a Raleigh-Ritz like formulation. In the process, we establish the manner of effect of the drift and any inducing potential on the size of the principal eigenvalue. We show that the degree of convexity of the potential plays a major role in this regard.

Key words: Fokker-Planck Equation, Indefinite Potential, Principal Eigenvalue.

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1. Introduction

In the absence of randomness, the directed motion of a particle on the real line due to an existing differentiable potential $B(x, t)$ (see [17]) is given by

$$\frac{dx}{dt} = \frac{\partial B}{\partial x} = b(x, t). \quad (1.1)$$

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The drift function $b(x, t)$ is then the velocity with which the particle travels, and in the event that B does not vary with time, the motion of the particle is steady and satisfies the equation

$$x(t) - B(x(t)) = c. \quad (1.2)$$

Assuming an additional random component for the motion of the particle without violating its continuity, equation (1.1) can be expanded to the Langevin equation:

$$dx(t) = b(x, t) + s(x, t)\Phi(t)dt. \quad (1.3)$$

Here, the function $\Phi(t)$ is rapidly fluctuating with time, having null statistical mean and Dirac δ variance function. The quantity $\Phi(t)dt$ is commonly known to be closely related to the Wiener process $w(t)$ (see [13]). The function $s(x, t)$ indicates the scale of randomness in the particle motion and is connected with the phenomenon of diffusion in the prescribed medium (see [9]). In fact, the diffusion coefficient of the medium $D(x, t)$ is known to be given by the relation:

$$D(x, t) = \frac{s^2(x, t)}{2}. \quad (1.4)$$

Clearly, $D(x, t)$ is a nonnegative function, and in this regard the Langevin equation may technically be called the stochastic drift-diffusion equation, and be written:

$$dx(t) = b(x, t)dt + \sqrt{2D(x, t)}dw(t). \quad (1.5)$$

The problem at hand is to estimate the influence of the drift $b(x, t)$ on the behavior of the particle motion described by the Langevin equation in a finite interval $[s_1, s_2]$ having absorbing ends. Assuming that the particle is subjected to a reactive potential $m(x, t)$ that changes sign in the interval $[s_1, s_2]$, we may ask how is the long term behavior of the particle affected if the drift is induced by $m(x, t)$. The standing conjecture (see [2, 5]) is that for the reflecting barrier case a drift along m_x should settle the particle mostly in areas where the potential m is optimally positive. This is treated in [6]. Here, we only consider the absorbing barrier case.

2. Stratonovich Versus Itô Integration

Techniques for solving stochastic equations like (1.5) depart greatly from those for solving ODEs. In this regard, the authors of [11] state that: *The stochastic nature of the Langevin equation allows an infinite number of possible trajectories for any given initial conditions. The probability of any one trajectory is governed by the statistical properties of the randomly fluctuating force.* The value of equation (1.5) comes from our ability to integrate it when possible. Integrating (1.5) in the interval $[s_1, s_2]$ yields:

$$x(s_2) - x(s_1) = \int_{s_1}^{s_2} bdt + \int_{s_1}^{s_2} \sqrt{2D(xt)}dw(t). \quad (2.1)$$

The first integral in the previous equation is a Riemann-Stieltjes one, and it may be calculated by rules of ordinary calculus, while the second integral is stochastic in nature. Given a continuous, nonanticipating function $f(t)$ (see [13]), and a partition $s_1 = t_0 < t_1 < \dots < t_n = s_2$ of the interval $[s_1, s_2]$, we choose τ_i 's such that $t_{i-1} \leq \tau_i \leq t_i$ and compute the sequence of partial sums:

$$S_n = \sum_{i=1}^n f(\tau_i) [\omega(t_i) - \omega(t_{i-1})]. \quad (2.2)$$

The value of S_n depends greatly on how the τ_i 's are chosen and on the value of $f(\tau_i)$. If we set $\tau_i = \alpha t_{i-1} + (1 - \alpha)t_i$, $0 \leq \alpha \leq 1$, then $S_n = S_n(\alpha, f, s_1, s_2)$. The stochastic integral of f may be defined in the following manner:

$$I(\alpha, f, s_1, s_2) = \int_{s_1}^{s_2} f(t) d\omega(t) = ms \lim_{n \rightarrow \infty} S_n(\alpha, f, s_1, s_2), \quad (2.3)$$

where ms means the limit in the mean square (L^2 norm). The $\widehat{\text{Ito}}$ stochastic integral is given by:

$$I(1, f, s_1, s_2) = ms \lim_{n \rightarrow \infty} S_n(1, f, s_1, s_2). \quad (2.4)$$

The Stratonovich stochastic integral, on the other hand, is given by:

$$I\left(\frac{1}{2}, f, s_1, s_2\right) = \int_{s_1}^{s_2} f(t) d\omega(t) = ms \lim_{n \rightarrow \infty} S_n\left(\frac{1}{2}, f, s_1, s_2\right). \quad (2.5)$$

We remark that for $f(t) \equiv 1$, $I(1, f, s_1, s_2) = I\left(\frac{1}{2}, f, s_1, s_2\right)$, while

$$I(1, \omega(t), s_1, s_2) = \frac{1}{2} [\omega^2(t) - t]_{s_1}^{s_2}, \quad (2.6)$$

and

$$I\left(\frac{1}{2}, \omega(t), s_1, s_2\right) = \frac{1}{2} [\omega^2(t)]_{s_1}^{s_2}. \quad (2.7)$$

Note that the Stratonovich integral looks more like the regular Riemann integral and the term $[t]_{s_1}^{s_2} = (s_2 - s_1)$ that occurs in the $\widehat{\text{Ito}}$ formulation does not show up in the Stratonovich model. While the $\widehat{\text{Ito}}$ integral may be mathematically and technically more satisfactory, the Stratonovich quadrature may naturally be a better choice physically. Despite these discrepancies, it can be easily shown (see [1, 2]) that both approaches yield $(d\omega(t))^\delta = 0$ if $\delta > 2$, and $(d\omega(t))^2 = dt$ in the mean square.

3. Stratonovich Versus $\widehat{\text{Ito}}$ Dynamical Model Formulation

For developmental and historical reasons, the stochastic equation (1.5) describing a Markov process (See [14, 18]) has become to be known as the $\widehat{\text{Ito}}$ Differential Equation (IDE):

$$dx(t) = bdt + \sqrt{2D}d\omega(t). \quad (3.1)$$

Another rival model to the IDE also describing particle motion due to drift and diffusion is given by the Stratonovich Differential Equation (SDE):

$$dx(t) = \left[b - \frac{D_x}{2}\right]dt + \sqrt{2D}d\omega(t). \quad (3.2)$$

$\widehat{\text{Ito}}$ and Stratonovich formulations are identical if the diffusion D is independent of the location. It is shown by the authors of [19] that both, the IDE (3.1) and the SDE (3.2), can lead to natural solutions. Here among other results, we develop their ideas further. The $\widehat{\text{Ito}}$ change of variable formula is given by (see [1] for a proof):

$$\begin{aligned} df(x(t)) &= [bf'(x(t)) + Df''(x(t))]dt + \sqrt{2D}f'(x(t))d\omega(t) \\ &= f'(x(t))dx(t) + Df''(x(t))dt. \end{aligned} \quad (3.3)$$

On the other hand, the Stratonovich chain rule is that of ordinary calculus as can be seen from the next result.

Theorem 3.1: *For a differentiable function f of $x(t)$ given by the SDE (3.2),*

$$df(x(t)) = f'(x(t))dx(t). \quad (3.4)$$

Proof: We start with the SDE:

$$dx = b^S dt + \sqrt{2D}d\omega(t). \quad (3.5)$$

This equation may be converted into an IDE as follows:

$$dx(t) = \left[b^S + \frac{D_x}{2}\right]dt + \sqrt{2D}d\omega(t). \quad (3.6)$$

Now, letting $y = f(x)$ gives rise to the inverse $x = g(y)$, with

$$\left(\frac{dg}{dy}\right)^{-1} = \frac{dy}{dg} = \frac{df}{dx}.$$

Furthermore, we have $D(x) = D(y)$ and $b^S(y) = b^S(x)$. After substitutions of these equalities, and manipulations of the IDE, we get:

$$dy = \left[b^S \left(\frac{dg}{dy}\right)^{-1} + D_y \left(\frac{dg}{dy}\right)^{-2} - D \frac{d^2g}{dy^2} \left(\frac{dg}{dy}\right)^{-3}\right]dt + \sqrt{2D} \left(\frac{dg}{dy}\right)^{-1} d\omega(t). \quad (3.7)$$

Now, we convert this IDE back to an SDE and obtain:

$$df(x) = dy = \left[b^S dt + \sqrt{2D}d\omega(t)\right] \left(\frac{dg}{dy}\right)^{-1}. \quad (3.8)$$

Using the previous defining relations, we recover the theorem conclusion.

It was shown (see [1, 6]) that a Langevin particle subject to diffusion $D(x, t)$ and to drift $b(x, t)$, hence governed by the IDE (3.1), resulting in the probability density $p(x, t)$ evaluating the chances of the particle being at location x at every time t , and a probability flux:

$$J(x, t) = b(x, t)p(x, t) - \frac{\partial}{\partial x}[D(x, t)p(x, t)]. \quad (3.9)$$

It must satisfy the Fokker-Planck Equation (FPE):

$$\frac{\partial p}{\partial t} = -\frac{\partial}{\partial x}J = \frac{\partial}{\partial x}\left[\frac{\partial}{\partial x}(Dp) - bp\right]. \quad (3.10)$$

The next result establishes the correct form of the FPE due to a Stratonovich drift.

Theorem 3.2: *Assuming that the Langevin particle moves under the influence of a Stratonovich drift $b^S(x, t)$ yields the corresponding FPE:*

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x} \left[\sqrt{D} \frac{\partial}{\partial x} (\sqrt{D} p) - b^S p \right]. \quad (3.11)$$

Proof: Since $b^S = b - \frac{D_x}{2} = b - ss_x$, where b is the $\hat{I}$ to drift, we see that the FPE (3.10) can lead to

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x} \left[\frac{\partial}{\partial x} (Dp) - bp \right] = \frac{\partial}{\partial x} \left[D \frac{\partial p}{\partial x} + \frac{D_x}{2} p - (b - \frac{D_x}{2}) p \right]. \quad (3.12)$$

Exchanging $\frac{s^2}{2}$ for D we get:

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x} \left[\frac{s^2}{2} \frac{\partial p}{\partial x} + \frac{ss_x}{2} p - b^S p \right] = \left[\frac{s}{\sqrt{2}} \frac{\partial}{\partial x} \left(\frac{s}{\sqrt{2}} p \right) - b^S p \right]. \quad (3.13)$$

Substituting $\sqrt{D}$ for $\frac{s}{\sqrt{2}}$ in equation (3.13) we get the Stratonovich FPE (3.11).

Clearly, both formulations coincide if diffusion is isotropic; $D(x) = D = \text{constant}$. Moreover, both equations (3.10) and (3.11) are valid in the absence of reactions. In the next section, we treat reactive versions of the FPEs with constant diffusion. In the absence of drift, equations (3.1) and (3.5) lead to the heat equation versions of (3.10) and (3.11) (see [10, 12, 18]). Introduction of drift into the FPEs helped explain many cellular dynamic phenomena (see, for instance, [3, 4, 9, 21]).

4. Indefinite Reactions Effects on the Dynamics of a Langevin Particle

In this section, we treat the isotropic case of a Langevin particle subject to a T -periodic drift $b(x, t)$ and a T -periodic indefinite reactive potential $m(x, t)$. We seek a probability density function $p(x, t)$ to the T -periodic parabolic eigenvalue problem

$$\frac{\partial p}{\partial t} - \frac{\partial}{\partial x} \left[D \frac{\partial p}{\partial x} - bp \right] = \lambda mp \text{ in } (s_1, s_2) \times [0, T], \quad (4.1)$$

with initial density $p_0 = p(x, 0)$, such that at all times, the given data at the boundary points s_1 and s_2 is $p = 0$. This means that we have Dirichlet conditions at the endpoints. The driftless problem with reflecting barriers at the endpoints ($\frac{\partial p}{\partial x} = 0$) was treated in [8]. Further developments including drift can be found in [3, 5, 6, 16]. Here, however, we focus on the Dirichlet case.

The recent results of [7] imply that under Dirichlet conditions, provided $\int_0^T \max_{[s_1, s_2]} (m(x, t) dt) > 0$, problem (4.1) admits a principal eigenvalue $\lambda^* > 0$ having a positive T -periodic density $p(x, t)$. An easy consequence of the previous statement shows that provided $\int_0^T \min_{[s_1, s_2]} (m(x, t) dt) < 0$, problem (4.1) admits a negative principal eigenvalue λ_* having a T -periodicity density $q(x, t)$. This can be easily seen by realizing that in problem (4.1), the quantity $\lambda mp = (-\lambda)(-m)p$. Both p and q are in $C^{2+\theta, 1+\frac{\theta}{2}}([s_1, s_2] \times \mathbb{R})$ if b and m are in $C^{1+\theta, 1+\frac{\theta}{2}}([s_1, s_2] \times \mathbb{R})$.

The next few results connect λ^* and p to the coefficients of the eigenvalue problem.

Theorem 4.1: *Let m and b be T -periodic in t , and let $b(x, t)$ be differentiable with respect to x , then the positive principal eigenvalue λ^* of problem (4.1) subject to Dirichlet*

conditions $(p(s_2, t) = p(s_1, t) = 0)$ is connected to the corresponding eigendensity function $p(x, t)$ by the following

$$\lambda^* \int_0^T \int_{s_1}^{s_2} m p^2 dx dt = D \int_0^T \int_{s_1}^{s_2} (p_x)^2 dx dt + \int_0^T \int_{s_1}^{s_2} \frac{b_x}{2} p^2 dx dt. \quad (4.2)$$

Proof: Multiplying problem (4.1) by p and integrating over $[s_1, s_2]$, we get:

$$\lambda \int_{s_1}^{s_2} m p^2 dx = \int_{s_1}^{s_2} J_x p dx + \int_{s_1}^{s_2} \frac{\partial p}{\partial t} dx \quad (4.3)$$

$$= \int_{s_1}^{s_2} [Jp]_x dx - \int_{s_1}^{s_2} J p_x dx + \int_{s_1}^{s_2} \frac{\partial p}{\partial t} dx.$$

Using Dirichlet boundary conditions, the first integral on the right-hand side vanishes, and the second integral yields:

$$- \int_{s_1}^{s_2} J p_x dx = D \int_{s_1}^{s_2} (p_x)^2 dx + \int_{s_1}^{s_2} \frac{b_x}{2} p^2 dx. \quad (4.4)$$

Therefore, we have

$$\lambda \int_{s_1}^{s_2} m p^2 dx = D \int_{s_1}^{s_2} (p_x)^2 dx + \int_{s_1}^{s_2} \frac{b_x}{2} p^2 dx + \int_{s_1}^{s_2} \frac{\partial p}{\partial t} dx. \quad (4.5)$$

Integrating equation (4.5) on interval $[0, T]$, we obtain:

$$\int_0^T \int_{s_1}^{s_2} \frac{\partial p}{\partial t} dx dt = \int_{s_1}^{s_2} \int_0^T \frac{\partial p}{\partial t} dt dx = \int_{s_1}^{s_2} [p(x, t)]_0^T dx \equiv 0. \quad (4.6)$$

Since $p(x, t)$ is T -periodic, we get:

$$\lambda \int_0^T \int_{s_1}^{s_2} m p^2 dx dt = D \int_0^T \int_{s_1}^{s_2} (p_x)^2 dx dt + \int_0^T \int_{s_1}^{s_2} \frac{b_x}{2} p^2 dx dt. \quad (4.7)$$

So that if $\lambda = \lambda^*$, p is the corresponding eigendensity.

Remarks: Similarly if $\lambda = \lambda_*$, then $p = q$. Also, note that if we denote $\lambda^* = \lambda(D, b, m)$, we see that $\lambda(D, b = \text{constant}, m) = \lambda(D, 0, m)$. In other words, a constant drift in $[s_1, s_2]$ has no effect on the value of the eigenvalue λ^* (nor on the value of λ_*). This is due to the fact that λ^* is the smallest nonnegative eigenvalue of problem (4.1).

In the next results, we consider the situation where for real α ,

$$b = \alpha \frac{\partial m}{\partial x}. \quad (4.8)$$

Corollary 4.2: Let m and b in Theorem 4.1 be related through equation (4.8). Then:

$$\lambda^* \int_0^T \int_{s_1}^{s_2} m p^2 dx dt = D \int_0^T \int_{s_1}^{s_2} (p_x)^2 dx dt + \frac{\alpha}{2} \int_0^T \int_{s_1}^{s_2} m_{xx} p^2 dx dt. \quad (4.9)$$

Proof: Clearly if b is related to m through relation (4.8), then:

$$b_x = \alpha \frac{\partial^2 m}{\partial x^2}. \quad (4.10)$$

Substituting this in equation (4.7) yields the desired result.

Equation (4.9) shows that the principal eigenvalue λ^* is influenced by the degree of concavity or convexity of the potential $m(x, t)$. The next result is concerned with the influence of the drift b and weight m on the eigenvalue λ^* (and λ_*) in the steady case (long term behavior).

Corollary 4.3: In the steady state case with $b = b(x)$, $m = m(x)$, we have $p = p(x)$ and

$$\lambda^* \int_{s_1}^{s_2} m p^2 dx = D \int_{s_1}^{s_2} (p_x)^2 dx + \int_{s_1}^{s_2} \frac{b_x}{2} p^2 dx. \quad (4.11)$$

Furthermore, if b and m are related via equation (4.8), then

$$\lambda^* \int_{s_1}^{s_2} m p^2 dx = D \int_{s_1}^{s_2} (p_x)^2 dx + \frac{\alpha}{2} \int_{s_1}^{s_2} m_{xx} p^2 dx. \quad (4.12)$$

Proof: Equations (4.11) and (4.12) are obtained from (4.2) and (4.9) respectively, by the obvious substitution, for the Dirichlet eigenvalue problem in (s_1, s_2) :

$$-\frac{\partial}{\partial x} \left[D \frac{\partial p}{\partial x} - b p \right] = \lambda m p, \quad (4.13)$$

considered periodic-parabolic for every period $T > 0$.

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