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Brownian motion and its descendants according to Schrödinger

Piotr Garbaczewski [1] and Jean-Pierre Vigier
Laboratoire de Physique Théorique, Institut Henri Poincaré, Université Paris VI, 11 Rue Pierre et Marie Curie, 75231 Paris Cedex 05, France

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We revisit Schrödinger's original suggestion of the existence of a special class of random processes, which have their origin in the Einstein–Smoluchowski theory of Brownian motion. Our principal goal is to clarify the physical nature of links connecting the realistic Brownian motion with the abstract mathematical formalism of Nelson and Bernstein diffusions.

The original analysis [1] due to Schrödinger of the probabilistic significance of the heat equation and of its time adjoint in parallel remained unnoticed by the physics community and since then has been forgotten. It reappeared however in the mathematical literature [2–5] as an inspiration to generalize the concept of Markovian diffusions to the case of Bernstein stochastic processes. But, without consequences for a deeper understanding of possible physical phenomena, which might underlie the corresponding abstract formalism.

Schrödinger's objective was to initiate investigations of possible links between quantum theory and the theory of Brownian motion, an attempt which culminated later in the so-called Nelson's stochastic mechanics [6,7] and its encompassing formalism of refs. [8–10] in which the issue of the Brownian implementation of quantum dynamics is placed in the framework of Markov–Bernstein diffusions (see refs. [11–13]).

Schrödinger's discussion [1] of the analogy between wave mechanics and random phenomena of classical statistical physics, starts with recalling an obscurity present in the notion of probability (Born's postulate) adopted in quantum theory. For the purposes of the probabilistic interpretation it seems that one should decide in advance whether one is considering a probability *after* one knows what has happened or rather a probability of what *is to happen*.

The quantum mechanical density $\rho(x, t) = (\psi\bar{\psi})(x, t)$ follows from introducing two symmetrical systems of ψ-waves propagating in the opposite directions of time. Therefore (Eddington, cited in ref. [1]): "one of these must presumably correspond to probable inference from what is known (or is stated) to have been the condition at a later time".

To conform with the classical notion of probability (an event i.e. sample space is needed to define the probability space of the axiomatic definition) the most natural way is to look at a classical probabilistic system, which structurally is as close as possible to the wave (Schrödinger) equation of quantum mechanics. In case of free ($V=0$) propagation, the heat equation with its time adjoint well fits the purpose:

$$\begin{array}{lcl} \mathrm{i}\partial_t\psi = -D\triangle\psi & & \partial_t\theta_* = D\triangle\theta_*\,, \\ & \overset{t\to \mathrm{i}t}{\longleftrightarrow} & \\ \mathrm{i}\partial_t\bar{\psi} = D\triangle\psi & & \partial_t\theta = -D\triangle\theta\,, \end{array} \qquad (1)$$

where the familiar imaginary time transformation is indicated as the recipe to pass from quantum theory to statistical physics.

Here ψ, $\bar{\psi}$ are complex while θ_*, θ are real functions and the diffusion constant D is left unspecified ($D=\hbar/2m$ gives rise to the Schrödinger equation in its standard form).

Let us now consider, basically following Schrödinger [1] and Jamison [5], the transition probability

[1] On leave of absence from: Institute of Theoretical Physics, University of Wrocław, PL-50-205 Wrocław, Poland.

density (heat kernel) $h(x, s, y, t)$ for the Brownian motion $\{Y_t, t_1 \leqslant t \leqslant t_2\}$ on an interval $[t_1, t_2]$, i.e.

$$h(x,s,y,t) = [4\pi D(t-s)]^{-1/2} \exp\left(-\frac{(y-x)^2}{4D(t-s)}\right), \tag{2}$$

where Y_t takes values in $\mathbb{R}^1$ (Brownian motion in one spatial dimension).

If we prescribe the initial particle distribution $\rho_1(x)$ for the random variable Y_{t_1} then all intermediate distributions of $\{Y_t, t_1 \leqslant t \leqslant t_2\}$ are determined in terms of $\rho_1(x)$ and $h(x, s, y, t)$ including the terminal one as well. We have indeed

$$\rho(x,t) = \int h(z, t_1, x, t)\rho_1(z)\,\mathrm{d}z\,, \quad t \geqslant t_1\,. \tag{3}$$

Starting from the classical Brownian law of random displacements (2) we can ask the following question: *Assuming that a test particle originates from x_1 at t_1 and terminates its route in (about) x_2 at t_2, what is the probability to find it in-between x and $x+\Delta x$ at the intermediate time t, $t_1 < t < t_2$?*

The pertinent intermediate probability distribution is given [1] by the conditional transition probability density formula (identified as the Bernstein transition density in refs. [5,8–10]

$$\rho(x,t) = P(x_1, t_1; x, t; x_2, t_2) = \frac{h(x_1, t_1, x, t)h(x, t, x_2, t_2)}{h(x_1, t_1, x_2, t_2)}\,. \tag{4}$$

It is then obvious that this formula for $\rho(x, t)$ can always be rewritten as a product of the solutions $\theta(x, t)$ and $\theta_*(x, t)$ of the heat equation and its time adjoint $\rho(x, t) = (\theta\theta_*)(x, t)$ provided $t_1 < t < t_2$.

Let us now define $\rho(x, t_0) = \rho_0(x)$ and $\rho(x, T) = \rho_T(x)$ to be the initial and final probability distributions *determined* by the Bernstein transition density (4) with $t_1 < t_0 < T < t_2$. Although we know the general Brownian transition mechanism (the law of random displacements) as given by (2), the *conditioning* present in (4) allows one to formulate a *new* probabilistic problem. In fact we are now revisiting Schrödinger's original question [1,5,13], i.e.: *What is the most likely way for the particles to evolve as t goes from t_0 to T once we have prescribed in advance both the initial $\rho_0(x)$ and terminal $\rho_T(x)$ probability densities for the process (given the prior transition mechanism (2))?*

The answer is given by deriving from the original (prior) process $\{Y_t, t_1 < t < t_2\}$ a new one $\{X_t, t_1 < t_0 \leqslant t \leqslant T < t_2\}$, which is presently known as the Markov–Bernstein process [8–10]. Two remarks can be made immediately.

Remark 1. The above discussion can be rephrased in more phenomenological terms. Suppose that the observer is measuring a coordinate x of the event (a particle entering the observation area A, the measurement accuracy does not matter) at time t_0 viewed as the initial time in a repeatable series of one-particle experiments. Accumulating the data one arrives at the empirical distribution, which asymptotically is found to approximate a probability distribution $\rho_0(x)$. It is then taken to characterize the "state of the system" at time t_0.

Assume also that the observer is collecting the coordinate data of these repeatable events (entering particles) in the detection area B at a later time T. Let them approximate the terminal probability distribution $\rho_T(x)$. If $\rho_T(x)$ is far from what it should be according to the law of large numbers (i.e. when $\rho_T(x)$ is much different from $\int \mathrm{d}y\, h(x, t_0, y, T)\rho_0(y)$, with h given by (2)), then we arrive at the *core* of the original Schrödinger discussion: *What are the intermediate probability distributions $\rho(x, t)$ and what is the particular transition mechanism responsible for the probabilistic evolution from $\rho_0(x)$ to $\rho_T(x)$ if no external forces are affecting the particle except for the Brownian noise?*

Remark 2. The stochastic process connecting $\rho_0(x)$ with $\rho_T(x)$ is Markovian, if and only if $\rho_0 = \theta_0\theta_{*0}$ and $\rho_T = \theta_T\theta_{*T}$ holds, where the functions $\theta_i(x)$, $\theta_{i*}(x)$ $(i=0, T)$ come out as the boundary data for solutions of the (dual) heat equations (1). Then, the transition probability densities for the Markovian (interpolating) diffusions are defined as follows [8–10],

$$p(x,s,y,t) = h(x,s,y,t)\,\frac{\theta(y,t)}{\theta(x,s)}\,,$$

$$p_*(x,s,y,t) = h(x,s,y,t)\,\frac{\theta_*(x,s)}{\theta_*(y,t)}\,,$$

$$t_0 \leqslant s < t \leqslant T\,. \tag{5}$$

h is given by (2), p is the forward and p_* the backward transition density of the interpolating diffusion process.

Let us stress that if the role of $p(x, s, y, t)$ is to allow for statistical predictions about the future, given the present $\rho(y, t)=\int p(x, s, y, t)\rho(x, s)\,dx$, then $p_*(x, s, y, t)$ allows one to reproduce the past statistical data of the process, given the present $\rho(x, s)=\int p_*(x, s, y, t)\rho(y, t)\,dy$, $s<t$. If, in case of repeatable processing with single (sample) Brownian particles, $p(x, s, y, t)$ represents a microscopic transport mechanism for the diffusion process, then quite on the contrary, the backward "transport" executed by means of $p_*(x, s, y, t)$ is merely a mathematical device allowing one to reveal the statistical history preceding the present data. Such a process should not be confused with any realistic particle transport going opposite to the time arrow.

Let us proceed with the further analysis as follows. The Bernstein transition density (4) plays a fundamental role in the stochastic process construction of refs. [2–5,8–10]. Once the moments $t_1<t_0<T<t_2$ are fixed and the primary transition mechanism (h of (2)) is known, then the particular form of the boundary probability distributions $\rho_0(x)$, $\rho_T(x)$ is uniquely determined by the choice of the boundary points x_1 and x_2: they are the endpoints of the Bernstein "bridge" to be travelled in the time interval $[t_1, t_2]$. All intermediate densities $\rho(x, t)$, $t_0<t<T$, are then uniquely determined as well.

It thus appears that Schrödinger's problem of deducing a probabilistic evolution from $\rho_0(x)$ to $\rho_T(x)$ requires the identification of an appropriate "bridge", i.e. x_1, t_1 and x_2, t_2, as a substantial ingredient.

This can be applied to specific situations induced by the conventional Brownian motion.

Case 1. Following ref. [8] we can ask for a probabilistic interpolation between the coinciding boundary distributions:

$$\rho(x, t_0)=\rho(x, T)=\left(\frac{\alpha}{2\pi D(\alpha^2-\beta^2)}\right)^{1/2}\exp\left(-\frac{\alpha x^2}{2D(\alpha^2-\beta^2)}\right) \tag{6}$$

in the time interval $[t_0, T]$.

As emphasized in ref. [8], no physicist would expect such an evolution while having the traditional picture of the Brownian motion in memory. However (6) immediately follows from (2), (4). Indeed, let us set $t_0=-\beta=-T$ and $t_1=-\alpha=-t_2$, $0<\beta<\alpha$ and choose $x_1=0$ as a source of particles. If we confine attention to these Brownian particles only, which after a time 2α from their emission are bound to be back at (or at least not far away from) the initial location $x_1=0=x_2$, then (4) reduces to

$$\rho(x, t)=\left(\frac{\alpha}{2\pi D(\alpha^2-t^2)}\right)^{1/2}\exp\left(-\frac{\alpha x^2}{2D(\alpha^2-t^2)}\right)$$
$$=(8\pi D\alpha)^{1/2}h(0, -\alpha, x, t)h(x, t, 0, \alpha)\,, \tag{7}$$

where the transition densities

$$h(0, -\alpha, x, t)=[4\pi D(t+\alpha)]^{-1/2}\exp\left(-\frac{x^2}{4D(t+\alpha)}\right),$$

$$h(x, t, 0, \alpha)=[4\pi D(\alpha-t)]^{-1/2}\exp\left(-\frac{x^2}{4D(\alpha-t)}\right) \tag{8}$$

solve the system of heat equations in duality (1) in the time interval $[-\alpha, \alpha]\ni t$. The Bernstein "bridge" which induces the boundary data (6) is thus established and the forthcoming analysis of the process in terms of (5) becomes possible.

Case 2. Let us set $x_1=0$, $t_1=0$ in (4). Then

$$\rho(x, t)=\left(\frac{t_2}{4\pi D(t_2-t)t}\right)^{1/2}\times\exp\left(-\frac{x^2}{4Dt}-\frac{(x_2-x)^2}{4D(t_2-t)}+\frac{x_2^2}{4Dt_2}\right),\quad 0<t<t_2\,, \tag{9}$$

refers to the Bernstein "bridge" which comprises particles originating from the source $x_1=0$ at $t_1=0$ and whose destiny is to reach a terminal point x_2 after the flight time t_2.

Assume t to run over the interval $[0, T]$, $T\ll t_2$, and x_2 to be a distant spatial location (one can set $x_2=Vt_2$, with $|V|$ not too small). It is apparent that for such a terminal regime the Bernstein "bridge" *effectively* degenerates into the usual Brownian transition density

$$\rho(x, t)\simeq h(0, 0, x, t)\,,\quad x_2\ \text{large}\,,\quad t_2\gg T\,,\quad t\in[0, T]\,. \tag{10}$$

The infinite x_2, t_2 limit is under control here as well.

This tells us that if particles emanating from $x_1=0$ at $t_1=0$ are bound to reach a distant point x_2 after a sufficiently long flight time t_2, then their probability distribution $\rho(x, t)$ on a short (relative to t_2) time scale is given by the heat kernel (10).

We have thus created a situation where the Bernstein "bridge" effectively accounts for Brownian particles *outgoing from* $x_1=0$ at $t_1=0$ (while on their route towards a distant terminus x_2 to be reached at the remote time t_2).

Case 3. Quite analogously one arrives at the description of particles *incoming to* a terminal point x_2, when the Brownian source x_1 is distant enough and the flight time appropriately large. Indeed, the choice $x_2=0$, $t_2=0$ implying $t_1<t<0$, yields $(t-t_1=|t_1|-|t|,\ -t=|t|)$

$$\rho(x,t)=\left(\frac{|t_1|}{4\pi D|t|(|t_1|-|t|)}\right)^{1/2} \times \exp\left(-\frac{x^2}{4D|t|}-\frac{(x-x_1)^2}{4D(|t_1|-|t|)}+\frac{x_1^2}{4D|t_1|}\right). \tag{11}$$

If $|x_1|$ is sufficiently large and $t_1 \ll t<0$ we immediately arrive at the approximate formula (with a controllable infinite x_1, t_1 limit)

$$\rho(x,t)\simeq(4\pi D|t|)^{-1/2}\exp\left(-\frac{x^2}{4D|t|}\right) = h(x,t,0,0)\,. \tag{12}$$

Compare, e.g., (8) and account for $T<t<0$, $t_1 \ll T$. Formula (12) refers to the particles *incoming to* $x_2=0$, which originate from a distant Brownian source, at the remote emission moment t_1.

Remark 3. In case 2 the boundary distributions $\rho_0(x)$, $\rho_T(x)$ would reveal the *spreading* phenomenon, quite consistent with the standard intuitions. However, the exactly opposite (*shrinking*, implosion) effect arises in case 3, *which is by no means surprising* once the problem is analyzed in terms of Bernstein "bridges". While looking like a time reversal of the (irreversible according to the folklore understanding) Brownian evolution, it is simply a degenerate case of the Bernstein "bridge" with a distant source of particles, which are bound to reach a fixed terminal point.

If we have given transition probability densities characterizing a Markovian diffusion, then the drifts (local mean velocities) of the stochastic flow can be evaluated as follows [7,14]. We can write

$$b(x,t)\Delta t \simeq \int dy\, p(x,t,y,t+\Delta t)y - x\,,$$

$$b_*(x,t)\Delta t \simeq x - \int dz\, p_*(z,t-\Delta t,x,t)z\,, \tag{13}$$

where Δt is a small time increment, b is the forward (mean velocity of particles outgoing from x at t) while b_* is the backward (mean velocity of particles incoming to x at t) drift of the diffusion, $t_0 \leqslant t \leqslant T$. The drifts (13) stand [7] for the substitutes of time derivatives, non-existent [6,7] in the naive sense for Wiener paths. Here $(D_+X)(t)=b(x,t)$ is the left time derivative in the conditional mean, while $(D_-X)(t)=b_*(x,t)$ is the right one.

In case 1 both formulas (13) can be immediately evaluated by means of (5). Up to the irrelevant multiplicative constants we can set (θ_* refers to the forward, θ to the backward evolution (1))

$$\theta_*(x,t)\sim h(0,-\alpha,x,t)\,,$$

$$\theta(x,t)\sim h(x,t,0,\alpha)\,,\quad -\beta\leqslant t\leqslant\beta<\alpha\,, \tag{14}$$

and consequently (see, e.g., ref. [8]) there holds

$$b(x,t)=\frac{2D\nabla\theta}{\theta}=-\frac{x}{\alpha-t}=-\frac{x(\alpha+t)}{\alpha^2-t^2}=u+v\,,$$

$$b_*(x,t)=-\frac{2D\nabla\theta_*}{\theta_*}=\frac{x}{\alpha+t}=\frac{x(\alpha-t)}{\alpha^2-t^2}=-u+v\,. \tag{15}$$

We have here a natural decomposition into two terms, one of which (i.e. v) is odd, while the other (i.e. u) is even with respect to time reversal. Moreover (compare, e.g., the exponents in formulas (6), (8)) the following relations hold,

$$u=2D\nabla R\,,\quad v=2D\nabla S\,,$$

$$\frac{x^2}{4D(\alpha+t)}=R-S\,,\quad \frac{x^2}{4D(\alpha-t)}=R+S\,,$$

$$R=-\frac{\alpha x^2}{4D(\alpha^2-t^2)}\,,\quad S=-\frac{tx^2}{4D(\alpha^2-t^2)}\,,$$

$$\theta_*\sim\exp(R-S)\,,\quad \theta\sim\exp(R+S)\,,$$

$$\rho(x,t)=(\theta\theta_*)(x,t)\sim\exp(2R)$$
$$\rightarrow u=\frac{D\nabla\rho}{\rho}=2D\nabla R\,. \quad (16)$$

In the above v is called the current velocity, while u is called the osmotic one. The osmotic velocity is invariant under time reversal and is intimately related to the concept [6,15,16] of osmotic transport: $u=D\nabla\rho/\rho$. Indeed, a macroscopic intuition of the osmotic diffusion [15] tells us that if one has set a particle concentration (area of higher density) somewhere, then the Brownian noise induces an expansion of particles and a continual lowering of the concentration as a consequence. In fact, if the concentration is given by $\rho(x,t)$, then the purely osmotic (Brownian) escape rate of particles from the area of higher density is defined [15] by the amount crossing a given point per time Δt:

$$-D\nabla\rho(x,t)\Delta t=-u(x,t)\rho(x,t)\Delta t\,, \quad (17)$$

which implies that ρ is a solution of the heat equation $\partial_t\rho=D\Delta\rho$. Notice that the actual flow of escaping particles is opposite to u, hence proportional to $-u$.

This situation is drastically different from the one for flows consistent with the conditioning underlying case 1. Formula (15) tells us [14] that $b_*(x,t)$ is the mean velocity evaluated over all sample paths which reach the point x at time t, while $b(x,t)$ is the mean velocity evaluated over all sample paths which emanate from x at time t. The average flow through x at time t is thus

$$\tfrac{1}{2}(b+b_*)(x,t)=v(x,t)\,. \quad (18)$$

Let us compare this outcome with the degenerate case 2. Then $\theta_*(x,t)\sim h(0,0,x,t)=\rho(x,t)$ and there holds [8]

$$b(x,t)=0\,,\quad b_*(x,t)=-\frac{2D\nabla\theta_*}{\theta_*}=\frac{x}{t}\,, \quad (19)$$

so that

$$\tfrac{1}{2}(b+b_*)(x,t)=\tfrac{1}{2}b_*(x,t)=\frac{x}{2t}=-\frac{D\nabla\rho}{\rho}\,, \quad (20)$$

which is the well-known mean particle flow characterizing the standard Brownian motion. See, e.g., ref. [16] where the phase-space discussion of the issue is given.

In case 3 the roles of the drifts are reversed, and we get ($\theta\sim h(x,t,0,0)=\rho(x,t)$, $t<0$)

$$b(x,t)=\frac{2D\nabla\theta}{\theta}=\frac{x}{t}=-\frac{x}{|t|}\,,$$
$$b_*(x,t)=0\,, \quad (21)$$

so that

$$\tfrac{1}{2}(b+b_*)(x,t)=-\frac{x}{2|t|}=\frac{D\nabla\rho}{\rho}\,, \quad (22)$$

which is an exact reversal of the standard formula (20).

Let us recall that we refer to degenerate Bernstein "bridges" here, so that (20) is an average over particles emitted by a Brownian source at $t=0$ and bound to reach a distant terminus, while (22) is an average over particles coming from a distant Brownian source to a terminus $x=0$ to be reached at the time $t=0$.

If we take $\frac{1}{2}(b+b_*)(x,t)=v(x,t)$ as the general current velocity definition, which applies to the degenerate cases 2 and 3 as well (in ref. [16] we have derived the mean velocity $\langle u\rangle_x=v(x,t)=-D\nabla\rho/\rho=-u(x,t)$ by phase-space arguments), we observe [14,8] that this implies

$$\partial_t\rho=-\nabla(\rho v)\,,\quad \partial_t v+v\nabla v=-\nabla Q\,,$$
$$Q=\frac{2D^2\Delta\rho^{1/2}}{\rho^{1/2}}\,, \quad (23)$$

whenever $\rho(x,t)$ has the form (4), degenerate cases included. The momentum balance equation (second equation in (23)) is an equivalent expression for Nelson's stochastic acceleration formula $\frac{1}{2}m(D_+D_++D_-D_-)X(t)=0$ (see, e.g., refs. [8–10] and refs. [6,7] for a further discussion).

An extension of the above analysis to more complex statistical problems (Bernstein "bridge" implemented interference of Brownian flows) and to the possible Brownian origin [16] of the stochastic (Nelson's) reformulation of quantum mechanics will be a subject of a subsequent paper.

Appendix

Let us observe that for a Bernstein "bridge" (4) with arbitrary finite spacetime endpoints x_1, t_1 and x_2, t_2 the choice of the new spatial coordinate origin at $\frac{1}{2}(x_1+x_2)$ and the shift of the time scale origin to the point $\frac{1}{2}(t_1+t_2)$ allows one to replace (4) by the fully symmetric expression (when written in relative coordinates)

$$x_1=-x_2=-X\,,\quad t_1=-t_2=-T\,, \tag{A.1}$$

where

$$\begin{aligned}\rho(x,t)&=P(-X,-T;x,t;X,T)\\&=[4\pi D(T^2-t^2)]^{-1/2}(2T)^{1/2}\exp\left(\frac{x^2}{2DT}\right)\\&\times\exp\left(-\frac{(X+x)^2(T-t)+(X-x)^2(T+t)}{2D(T^2-t^2)}\right)\end{aligned} \tag{A.2}$$

and

$$\begin{aligned}h(-X,-T,x,t)&=[4\pi D(t+T)]^{-1/2}\\&\times\exp\left(-\frac{(x-X)^2(T-t)}{4D(T^2-t^2)}\right),\\h(x,t,X,T)&=[4\pi D(T-t)]^{-1/2}\\&\times\exp\left(-\frac{(X-x)^2(T+t)}{4D(T^2-t^2)}\right),\end{aligned} \tag{A.3}$$

which in case of $X=0$ reduces to the previously considered example (6)–(8). By defining

$$\begin{aligned}\rho(x,t)&=(\exp 2R)(x,t)\,,\\S(x,t)&=\tfrac{1}{2}\ln\left(\frac{h(x,t,X,T)}{h(-X,-T,x,t)}\right)\end{aligned} \tag{A.4}$$

we realize that

$$\rho(x,t)=(\theta\theta_*)(x,t)\,. \tag{A.5}$$

Here the solutions of the dual system (1) have the form

$$\begin{aligned}\theta_*(x,t)&=\exp(R-S)\\&=(2T)^{1/4}\exp\left(\frac{X^2}{4DT}\right)h(-X,-T,x,t)\,,\\\theta(x,t)&=\exp(R+S)\\&=(2T)^{1/4}\exp\left(\frac{X^2}{4DT}\right)h(x,t,X,T)\,,\\R(x,t)&=-\frac{(X+x)^2(T-t)+(X-x)^2(T+t)}{8D(T^2-t^2)}\\&+\frac{X^2}{4DT}+\tfrac{1}{4}\ln\left(\frac{2T}{4\pi D(T^2-t^2)}\right),\\S(x,t)&=\frac{(X+x)^2(T-t)-(X-x)^2(T+t)}{8D(T^2-t^2)}\\&+\tfrac{1}{4}\ln\left(\frac{T+t}{T-t}\right),\end{aligned} \tag{A.6}$$

where the x-dependent contributions have a canonical form allowing one to demonstrate that

$$\begin{aligned}b_*(x,t)&=-\frac{2D\nabla\theta_*}{\theta_*}=-2D\nabla(R-S)\\&=(v-u)(x,t)\,,\\b(x,t)&=\frac{2D\nabla\theta}{\theta}=2D\nabla(R+S)\\&=(v+u)(x,t)\end{aligned} \tag{A.7}$$

consistent with Nelson's definition of the drifts in terms of the gradient (current and osmotic) velocity fields $u(x,t)$, $v(x,t)$.

Notice that the time reversal of (A.6) is accomplished by the simultaneous ($t\to -t$, $X\to -X$) mapping: the time label inversion is accompanied by the interchange of the spatial endpoints, the time scale endpoints are kept fixed.

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