Physical significance of the Nelson–Newton laws

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The mean acceleration formulas introduced by Nelson in his investigation of links between quantum theory and Markovian diffusions are necessary but insufficient conditions for a unique specification of the process. The resolution of Schrödinger’s probabilistic conjecture in terms of Markov–Bernstein processes and the related (induced) dynamical semigroups resolves this problem and sets the uniqueness criteria. We discuss the role of analytic time continuation in this formalism and demonstrate that on the appropriate level of description, the imaginary time transformation executes a mapping between two physically distinct families of Markovian diffusions, both proceeding in real time.

In the long history of investigations of possible links between quantum theory and the theory of Brownian motion, and more generally of Markov diffusion processes, a special role is played by the so-called Nelson stochastic mechanics [1,2], which aimed at establishing the definite equivalence principles between solutions of the Schrödinger equation and Markov diffusions. Although mathematically consistent it was criticised on physical grounds and especially the role of the mean acceleration formulas (we call them the Nelson–Newton laws) was at best disputable.

The original analysis [3] due to Schrödinger of the possible probabilistic significance of the heat equation in the quantum context (unfortunately unnoticed and forgotten since then) has inspired the generalisation [4,5], see also refs. [6,7] where another standpoint is favoured, which places the issue of the Brownian implementation of quantum dynamics in the framework of Markov–Bernstein processes. Then, Nelson’s formalism is derivable from first principles as one of the alternative realisations of the Schrödinger programme (Zambrini’s “Euclidean quantum mechanics” is another).

Although not explicit in the original formulations of stochastic mechanics, the kinetics theory description of the statistical ensemble dynamics is hidden behind the Nelson mean acceleration formulas.

We deal in fact with the Cauchy problem for the coupled system of nonlinear equations, which is composed of the probability conservation law

\[ \partial_t \rho = -\nabla (\rho v) \]  

and one of the momentum balance equations (we quite intentionally use the kinetic theory lore here)

\[ (\partial_s + v \nabla) v = \frac{1}{m} \nabla (V - Q) \]  \hspace{1cm} (Zambrini)  

or

\[ (\partial_s + v \nabla) v = \frac{1}{m} \nabla (Q - V) \]  \hspace{1cm} (Nelson)  

where (diffusions in one spatial dimension are considered throughout the paper for simplicity of arguments)

\[ Q = 2mD^2 (\Delta \rho^{1/2}) / \rho^{1/2} \]  

and \[ Q_s = -Q \] is immediately recognized as the familiar de Broglie–Bohm “quantum potential”. Its...
statistical origin in the present context was discussed elsewhere \[8—11\].

In the above formulation the initial data \(p_0(x), \ u_0(x)\) give rise to the purely deterministic evolution of \(p(x, t)\) and \(v(x, t)\). \(D\) is the diffusion constant, while \(V\) is the continuous potential of the conservative force field bounded from below.

If we introduce the mean local velocity field (forward drift of the diffusion process)

\[
b(x, t) = v(x, t) + D \frac{\nabla p}{p} = (v + u)(x, t),
\]

then the individual particle dynamics which might underlie either the system (1), (2) or (1), (3) is governed by the stochastic differential equation

\[
dX(t) = b(X(t), t) \, dt + \sqrt{2D} \, dW(t),
\]

where \(W(t)\) stands for the Wiener noise, while \(X(t)\) is the random variable of the diffusion process, interpreted as the idealised picture of position of the particle affected by the random environment at time \(t\) (usually belonging to a certain finite time interval \([t_0, T]\) whose boundaries under appropriate restrictions on the drift might be extended). Equation (6) is in fact the major assumption in the stochastic formalism devised by Nelson, since it explicitly takes the random sample path concept as the primordial entity in the theory. Accordingly, the random displacements are generated by the Wiener noise \(W(t)\), which superimposes probabilistic fluctuations upon the deterministic contribution \(b(x, t) \, dt\). The latter is a typical path ensemble input, since it includes the mean velocity evaluated over all sample paths originating from \(x\) at time \(t\), in the repeatable series of single particle trials: \(b(x, t)\) encodes the mean tendency of motion of individual members of the given (via the initial state preparation procedure) ensemble, which remains basically unidentifiable unless sufficiently many sample flight data are accumulated.

Via the stochastic Itô calculus eq. (6) implies the validity of the Kolmogorov (for the transition probability density of the process) and the Fokker–Planck equations. Since we have given the initial probability distribution \(p_0(x)\) its subsequent evolution is controlled by

\[
\partial_t p = D \Delta p - \nabla (bp), \quad p(x, t_0) = p_0(x),
\]

which in view of (6) coincides with (1). However (1) or (7) alone cannot be utilized to reconstruct the random dynamics in full detail. Indeed, if we assume the forward drift \(b(x, t)\) in (7) to be a priori given for all times of interest (like \(t \in [t_0, T]\)), then the forward transition probability density for short times in virtue of (7) takes the form

\[
p(y, t, x, t+\Delta t) \\ \approx (4\pi D \Delta t)^{-1/2} \exp \left( -\frac{[x - y - b(y, t) \Delta t]^2}{4D \Delta t} \right),
\]

\[0 < \Delta t \ll t,\]

and via the chain rule (with the Chapman–Kolmogorov equation consecutively utilized) gives rise to the standard path integral expression for the transition density,

\[
p(y, s, x, t) = \lim_{\Delta t \to 0} \int dz_1 \ldots \int dz_n (4\pi D \Delta t)^{-n/2} \\ \times \exp \left( -\frac{1}{4D \Delta t} \sum_{k=0}^{n-1} [z_{k+1} - z_k - b(z_k, t_k) \Delta t]^2 \right),
\]

\[
\Delta t = (t-s)/n, \quad z_0 = y, \quad z_n = x. \quad (9)
\]

Hence something specific must be assumed about the time development of \(b(x, t)\) to make the stochastic picture complete. There is no way to generate \(b(x, t+\Delta t)\) from the earlier data by means of the purely stochastic processing. For this purpose we must know \(\partial b = \partial_{\mu} + \partial_{\nu} \), \(\partial_{\mu}\) is provided by the Fokker–Planck equation for the density, \(\partial_{\mu} = -D \Delta v - V(uv)\), hence the only freedom left in the formalism to account for the random medium and particle response to external force fields pertains to \(\partial_{\nu}\).

By now it is well known that the only way to incorporate restrictions defining the dynamics of \(b(x, t)\), is through the formulas (we take here an apparent lesson from the original derivations of ref. \[5\] to present the Nelson–Newton laws in the form making explicit the induced semigroups intervention)

\[
D^2_+ X = D^2_- X = \frac{1}{m} \nabla V
\]

\[
\Rightarrow \frac{1}{2} (D_+ D_- + D_- D_+) X = \frac{1}{m} \nabla (V - 2Q) \quad (10)
\]

or
Markov—Bernstein process, which allows one to propagate (hence both predict the future and reproduce the past given the present) the probability distribution
\[ \tilde{\rho}(x, t) = \Theta(x, t) \Theta_\ast(x, t), \]
respectively forward and backward in time. Statistical predictions about the future can be accomplished by means of the forward transition probability density
\[ \tilde{\rho}(x, s, y, t) = h(x, s, y, t) \frac{\Theta(y, t)}{\Theta(x, s)}, \]
while the past can be reproduced statistically by means of the backward density
\[ \tilde{\rho}_\ast(x, s, y, t) = h(x, s, y, t) \frac{\Theta_\ast(x, s)}{\Theta_\ast(y, t)}, \]
for the diffusion with fixed boundary probability distributions \( \tilde{\rho}(x, -\frac{1}{2}T) \) and \( \tilde{\rho}(x, \frac{1}{2}T) \).

With \( \tilde{\rho} \) and \( \tilde{\rho}_\ast \) in hand, we can straightforwardly [8,9] evaluate the conditional expectation values, which are necessary to establish the mean forward and backward derivatives in time for functions of the random variable \( \tilde{X}(t) \in \mathbb{R}^1 \). The backward, \( (D_\ast \tilde{X})(t) = \tilde{b}_\ast(x, t) \), and forward, \( (D_+ \tilde{X})(t) = \tilde{b}(x, t) \), drifts of the Markovian diffusion (15), (16) read thus [4,5]
\[ \tilde{b}(x, t) = 2D \nabla \Theta / \Theta, \quad \tilde{b}_\ast(x, t) = -2D \nabla \Theta_\ast / \Theta_\ast, \]
so that the continuity equation follows,
\[ \tilde{v} = \frac{1}{2} (\tilde{b} + \tilde{b}_\ast), \]
\[ \partial_t \tilde{\rho} = -\nabla(\tilde{v} \tilde{\rho}) = D \Delta \tilde{\rho} - \text{div}(\tilde{b} \tilde{\rho}) = -D \Delta \tilde{\rho} - \text{div}(\tilde{b} \tilde{\rho}_\ast). \]

If we define \( \tilde{\Theta} = \exp(\tilde{R} + \tilde{S}) \) and \( \tilde{\Theta}_\ast = \exp(\tilde{R} - \tilde{S}) \), with \( \tilde{R}, \tilde{S} \) real functions, then there holds
\[ \tilde{v} = 2D \nabla \tilde{S}, \quad \tilde{u} = \frac{1}{2} (\tilde{b} - \tilde{b}_\ast) = 2D \nabla \tilde{R}, \]
and (17) can be rewritten as
\[ \frac{1}{2D} \partial_t \tilde{R} = -\frac{1}{2} \Delta \tilde{S} - (\nabla \tilde{R})(\nabla \tilde{S}) \quad \text{grad} \]
\[ \partial_t \tilde{u} = -D \Delta \tilde{u} - \nabla(\tilde{u} \tilde{v}), \]
the gradient form of (17) being due to Nelson [1,2]. If (17) (respectively (19)) holds, then the necessary consequence of (12) is [4–7]
\[ V = 2mD(\partial_s S + D(\nabla S)^2 + D[(\nabla R)^2 + \Delta R]), \]  
(20)

where (14) implies that
\[ 2mD^2[(\nabla R)^2 + \Delta R] = 2mD^2 \frac{\Delta \rho^{1/2}}{\rho^{1/2}} = \tilde{Q} \]  
(21)

holds. Except for the sign inversion \( \tilde{Q} \) has the familiar functional form of the Bohm–Vigier “quantum potential”, see e.g. ref. [10].

We can here argue in reverse (we adopt the stronger version of Nagasawa’s argument [6,7]): given (17) and (20) then the system (12) follows.

By evaluating the forward and backward time derivatives of \( \tilde{b}(x, t) \) and \( \tilde{b}_*(x, t) \) we can verify that the gradient form of (20),
\[ \partial_t \tilde{v} = 2D \Delta \tilde{u} + \frac{1}{2} \nabla \tilde{u}^2 + \frac{1}{2} \nabla \tilde{v}^2 + (1/m) \nabla V, \]  
(22)

implies the validity of the Nelson–Newton law with the (sign) inverted potential
\[ \frac{1}{2} m (D_+ D_+ + D_- D_-) \hat{X}(t) = \nabla V, \]  
(23)

which was primarily rejected by Nelson as the physically relevant characteristics of the Markovian diffusion (see e.g. ref. [11]).

Notice that (23) can be rewritten in the form
\[ (\partial_t + \nabla V) \tilde{v} = (-1/m) \nabla (\tilde{Q} - V) \]  
= (1/m) \nabla (V - \tilde{Q}), \]  
(24)

reminiscent of the momentum balance equation in the kinetic theory of gases and liquids, which should in principle apply to all conceivable osmotic diffusions (we are just dealing with one [10,11]).

Let us now introduce another pair of diffusion equations in duality,
\[ \partial_t \Theta_* = D \Delta \Theta_* - (2Q - V) \Theta_*/2mD, \]  
\[ \partial_t \Theta = -D \Delta \Theta + (2Q - V) \Theta/2mD, \]  
(25)

where \( V \) is the same as before, while \( Q = 2mD^2 \times (\Delta \rho^{1/2}) / \rho^{1/2} \) and \( \rho(x, t) = \Theta(x, t) \Theta_*(x, t) \) differ from the previously utilised objects by the absence of overbars, which is to distinguish solutions of (12) from those of (25).

All previous arguments can now be repeated by replacing the kernel \( k(x, s, y, t) \) of (12) by \( k(x, s, y, t) \) of (25). The transition probability densities (no overbar!) \( p \) and \( p_* \) respectively, allow one to arrive at the new drifts \( b(x, t) \) and \( b_*(x, t) \). The continuity equation in form (17) holds, \( \partial_t \rho = -\nabla (\rho v) \), and as a consequence of (25) we then arrive at the identity (compare with (20))
\[ 2Q - V = 2mD[\partial_s S + D(\nabla S)^2] + Q, \]  
(26)

where apparently
\[ (Q - V)/2mD = \partial_s S + D(\nabla S)^2 \]  
(27)

to be compared with (11). Here \( Q_0(x, t) = -Q(x, t) \) is identifiable as the previously mentioned Bohm–Vigier “quantum potential” [8,10].

Let us observe that the identity (26) implies
\[ 2Q = 2V + 4mD[\partial_s S + D(\nabla S)^2], \]  
(28)

which allows one to replace the system (25) by the equivalent one where the original potential \( V/2mD \) of (1) acquires a correction \( 2\partial_s S + 2D(\nabla S)^2 \).

While (23) was utilised by Zambrini [4,5], the system with the corrected potential was utilised by Nagasawa [6,7], however without notifying that the equivalence is established when the diffusions with creation and annihilation are replaced by Markov–Bernstein diffusions.

It is well known that the equations of continuity and (26) uniquely (Madelung representation) determine solutions of the Schrödinger equation
\[ 2imD \partial_x \psi = \left( -mD^2/2 \right) \Delta + V \psi, \]  
[psi(x, t) = \exp(R + iS)(x, t), \]  
(29)

but now solutions of the system (25) determine \( R \) and \( S \),
\[ R = \frac{1}{2} \ln(\Theta \Theta_*), \quad S = \frac{1}{2} \ln(\Theta/\Theta_*). \]  
(30)

For a discussion of the multiply connected (due to nodal surfaces) configuration space see ref. [5].

The previous argument holds also in reverse, since the standard Madelung route applies, and then we know that the continuity and Hamilton–Jacobi (26) equations imply [6,7] the coupled system of diffusion equations (25).

One immediately verifies that [5] the gradient form of (26) implies the Nelson–Newton law in the form
\[ \frac{1}{2} m (D_+ D_- + D_- D_+) \hat{X}(t) = -\nabla V, \]  
(31)
adopted by Nelson [1,2] to characterise diffusions underlying quantum mechanical phenomena.

Stochastic acceleration formulas play the role of momentum balance equations (in the mean!) for stochastic flows, and by finite difference arguments [9,12] they give an insight into random transport phenomena. However, the knowledge of gradient velocity fields $u, v$ ($\bar{u}, \bar{v}$, respectively) is insufficient for a unique reconstruction of the underlying stochastic theory. A good example is provided by Nelson’s own discussion (ref. [1], p. 100) of the harmonic oscillator ground state, where the expressions for the drifts read

\[
(D_+ X)(t) = -\gamma x, \quad (D_- X)(t) = \gamma x, \quad x = X(t),
\]

which allows one to evaluate

\[
\frac{1}{2}m(D_+ D_- + D_- D_+)X(t) = -m\gamma^2 x,
\]

\[
\frac{1}{2}m(D_+ D_+ + D_- D_-)X(t) = m\gamma^2 x,
\]

with the outcome that both Nelson–Newton laws seemingly apply to the same Schrödinger wave function. This obstacle generally appears in the discussion of quantum mechanical stationary states.

As well there is no obvious reason to postulate [1,2] the validity of (23) against (31) in case of freely diffusing particles, when

\[
\frac{1}{2}m(D_+ D_- + D_- D_+)X(t) = 0
= \frac{1}{2}m(D_+ D_+ + D_- D_-)\bar{X}(t),
\]

unless the acceleration formulas are derived from (12) and (25) instead of being postulated.

To exemplify the above discussion, let us take advantage of the $V=0$ analysis of ref. [10]. The solution

\[
\bar{\rho}(x, t) = (4\pi D t)^{-1/2} \exp\left(-\frac{x^2}{4Dt}\right)
\]

of the heat equation $\partial_\tau \bar{\rho} = D \partial_x^2 \bar{\rho}$ satisfies

\[
\bar{v} = -D \bar{\rho} \bar{\rho} = x/2t, \quad \bar{Q} = m(x^2/8t^2 - D/2t),
\]

\[
-\frac{1}{m} \nabla \bar{Q} = \frac{D}{2t} \bar{\rho} = -\frac{x}{4t^2} \quad \Rightarrow
\]

\[
\partial_\tau \bar{\rho} = -\nabla(\bar{\rho} \bar{v}), \quad (\partial_\tau + \bar{v} \nabla)\bar{v} = -\frac{1}{m} \nabla \bar{Q}.
\]

We have here the $V=0$ version of (1) and (2), so we are automatically led to the diffusion system (12), which evidently reduces to (23) once we define

\[
\Theta_\star = \exp(\bar{R} - \bar{S}) = \rho, \quad \Theta = 1 \quad \Rightarrow
\]

\[
\bar{R} = -\bar{S} = \ln(\rho^{1/2}).
\]

In this case the Markov–Bernstein process is irreversible and characterised by the backward drift \( \bar{h}_\star = -2D \bar{v} \Theta_\star / \Theta_\star \). The process coincides with the very traditional (Einstein–Smoluchowski) Brownian motion of particles originating at time $t=0$ from the source at $x=0$. Let us mention that in a different notation and with no special physical motivations, this example appears in section III of ref. [4].

The corresponding quantum mechanical problem

\[
i\partial_x \psi = -D \Delta \psi,
\]

\[
\psi(x, 0) = (\pi \alpha^2)^{-1/4} \exp\left(-\frac{x^2}{2\alpha^2}\right),
\]

refers to the $V=0$ version of (31) with

\[
\rho(x, t) = |\psi|^2(x, t)
= \frac{\alpha}{[\pi (\alpha^4 + 4D^2 t^2)]^{1/2}}
\times \exp\left[-\frac{x^2\alpha^2}{(\alpha^4 + 4D^2 t^2)}\right],
\]

\[
\psi(x, t) = 4D^2 t x / (\alpha^4 + 4D^2 t^2).
\]

The corresponding potentials $R$ and $S$ come from the explicit solution of the Schrödinger equation. With [10] a given forward transition probability density implying (39)

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

and knowing $R, S$ (hence $\Theta$ and $\Theta_\star$) one can easily reproduce the kernel $k$ and then $p_\star$, see formulas (15), (16), without overbars and $k$ instead of $\hbar$. This diffusion is a reversible process.

Let us consider the harmonic oscillator potential $V(x) = \frac{1}{2}m\gamma^2 x^2$. The ground state process of Nelson’s stochastic mechanics was identified in refs. [13–15] as the Markov process of the Euclidean (i.e. imaginary time) image of the harmonic oscillator, but an analysis in terms of (25) has never been performed. There is a real subtlety involved since solutions of the diffusion equations (12) and (25) quite sensitively depend [16–18] on the energy renormalisation: the operation $V \pm E$, $E$ being a constant, looks quite innocent from the point of view of
Nelson—Newton laws since \( V(V \pm E) = VV \). It has however quite dramatic consequences for the solutions of (12) and (25). This point was overlooked in refs. [14,15,4,5] where the gradient formulas were supposed to be sufficient to define the stochastic theory completely, while they are the necessary conditions for its derivation.

For quantum mechanical stationary states we have (via (28))

\[
2Q - V = V - 2E,
\]

\[
\psi(x, t) = \psi_0(x) \exp(-iEt/2mD).
\] (41)

Then for the once chosen potential \( V \) system (25) differs from system (12) merely by the additive renormalisation of the potential \( V \to V - 2E \). What are the consequences of such a change of the reference level for the potential on the stochastic processes involved?

It is well known (ref. [1], section I; ref. [17], theorem 1.5.10; ref. [18], ch. 5) that the Markov process of Nelson's stochastic mechanics, which is associated with the harmonic oscillator ground state

\[
\psi_0(x) = (\gamma/2\pi D)^{1/2} \exp(-\gamma x^2/4D)
\]

has [13,14,1] the forward transition probability density

\[
p(y, s, x, t) = (\gamma/2\pi D[1 - \exp(-2\gamma(t-s))]^{1/2} \times \exp\left(-\frac{\gamma(x-y) \exp(-\gamma(t-s))^2}{2D[1 - \exp(-2\gamma(t-s))]}\right),
\] (42)

which solves the forward Fokker–Planck equation [18,9]

\[
\partial_t p = D \Delta_x p - \nabla_x (bp) = D \Delta_x p + \gamma \nabla_x (xp),
\] (43)

where \( b(x, t) = -\gamma x \). It is however equally well known that the semigroup kernel \( k \) from which (via formulas (13)–(16)) the density can be derived is a solution of the diffusion equation

\[
\partial_t k = D \Delta_x k - (1/2mD)(V - E_0)k,
\]

\[
E_0 = mD\gamma.
\] (44)

Hence, on the basis of the previously outlined derivations, we have the following consistent choice of the Schrödinger equation,

\[
2imD \partial_x \psi = -\frac{1}{2} mD^2 \Delta \psi + (V + E_0) \psi,
\] (45)

as then only (45) would yield (44).

It however amounts to considering system (12) with \( V \to V + E_0 \) as the alternative to realisation (44) of the Schrödinger–Bernstein–Markov diffusion problem. The consequence is dramatic, since

\[
\partial_x h = D \Delta_x h - (1/2mD)(V + E_0)h
\] (46)

implies [18] the forward transition probability density

\[
\tilde{p}(y, s, x, t) = (\gamma/2\pi D[1 - \exp(-2\gamma(t-s))]^{1/2} \times \exp\left(-\frac{\gamma(x-y) \exp(-\gamma(t-s))^2}{2D[1 - \exp(-2\gamma(t-s))]}\right)
\]

\[
\times \exp(-\gamma(t-s)),
\] (47)

which solves \( \partial_t \tilde{p} = D \Delta_x \tilde{p} - \gamma \nabla_x (xp) \) and does not allow for stationary solutions at all.

Let us notice that we can pass from (42) to (47) by means of the \( \gamma \to -\gamma \) transformation, which to exploit the phase space derivation [19,10] of the Smoluchowski equation,

\[
\partial_t \tilde{p} = (\omega^2/\beta) \nabla_x (xp) + D \Delta \tilde{p},
\]

\[
g = \omega^2/\beta, \quad \beta \gg 2\omega, \quad t \gg \beta^{-1},
\] (48)

for a harmonically bound particle in a thermal bath, amounts to passing from the standard attractive harmonic potential to the inverted [20] (repulsive) one, \( \omega \to i\omega \Rightarrow \omega^2x^2 \to -\omega^2x^2 \), with obvious physical implications.

The above analysis justifies the correctness of Nelson's guess that the mean acceleration formula (20) is a necessary condition for the derivation of the diffusion process underlying Schrödinger wave mechanics, albeit it is not a sufficient condition: one must invoke (12) and (25) to resolve ambiguities. On the basis of the previous discussion (see also refs. [10,14,15]) we decline the intuition of imaginary time diffusions. Both considered Markov–Bernstein processes are undoubtedly the real time diffusions: the physically relevant distinction lies in the inversion of the mean accelerations for the stochastic flows. The imaginary time transformation (like the imaginary frequency transformation connecting two oscillator problems) on the appropriate level of description plays the role of the technical device map-
ping one diffusion into another, compare e.g. especially our $V=0$ discussion both in the present note and in ref. [10].

At the moment we leave aside the fundamental problem of the nature (origin and properties) of the random environment, whose material presence is indispensable on physical grounds [24], together with the possible phase-space implementation [10,21,25] of the configuration space diffusions. Some hints in the essentially probabilistic direction can be found in refs. [26–28], these linked to the kinetic theory concepts (hydrodynamical limit of the Boltzmann equation) in refs. [29,30]. The purely deterministic approach to the Brownian motion might be promising as well [31–33].

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References