

Quantum dynamics from the Brownian recoil principle

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We formulate a theory of the Brownian motion for particle ensembles, whose diffusive evolution is entirely generated by the surrounding random environment. By demanding the validity of the momentum conservation law on all conceivable scales adopted for the investigation of individual particle scattering (collisions) on the medium constituents, we are forced to incorporate the environmental recoil effects in the formalism. The Brownian recoil principle elevates the individually negligible phenomena to the momentum conservation law on the ensemble average. The resultant dynamics of the statistical ensemble is governed by the Schrödinger equation, once the diffusion constant D is identified with $\hbar/2m$.

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Nelson's stochastic mechanics [1] gives a persuasive stochastic insight into phenomena of exclusively quantum origin (Schrödinger wave mechanics). The resulting Markovian diffusions are, however, highly nonlinear diffusion processes, with an explicit dependence on the particle probability distribution mediated by the de Broglie-Bohm-Vigiér "quantum potential." For years its role was notoriously associated with the notion of the Einstein-de Broglie "pilot wave" capable of guiding micro-objects (e.g., particles) in space, so that the wave and particle features of the quantum dynamics could be to some extent simultaneously maintained. This is to be contrasted with Bohr's concept of the wave-particle duality.

Recent experiments [2] (mostly in the domain of neutron interferometry) suggest that if one extends the validity of energy-momentum conservation laws to the microscopic level, on which a detailed individual particle motion takes place, then the particle behaves as being under the influence of the nonlocal "quantum potential." On the other hand, the quantum potential itself *must* encode information about some realistic collective motions: particles appear to be members of statistical ensembles propagating in the totally chaotic (for us synonymous with random) environment. The problem of reconciling the individual and collective (ensemble) feature of such propagation has never, to the authors' knowledge, been convincingly addressed.

Our work can be considered as the natural extension of the Einstein and Smoluchowski pioneering investigations of the Brownian motion, where we consider as non-negligible (at least on the ensemble average) a reciprocal interaction (*recoil* effect) of particles being Brownian scattered by the random medium, with the medium itself.

For a very rough analogy with this situation, let us consider a substance (like, e.g., milk) whose constitutive elements undergo a completely chaotic (which might be Brownian as well) motion. Let us immerse a droplet of ink (one should rather think about individual ink molecules which are consecutively one by one implanted in

the medium according to some prescribed initial particle distribution) in milk, and assume that the ink elements will undergo the Brownian diffusion which is entirely generated by the chaotic medium and has nothing in common with the traditional picture of ink self-diffusion via its own molecular agitation. The idea of energy-momentum conservation on the individual (ink) particle level certainly must give rise to some reciprocal (recoil) effects in the random environment.

Further reasoning depends on the properties of the random environment, which one considers to be relevant to the problem. If one neglects such reciprocal phenomena, as Einstein did [3], the standard theory of Brownian motion emerges. If, however, one considers the *recoil* effects to affect random particle motions, then one ends up (as we wish to demonstrate) with the nonlinear diffusion of Nelson's stochastic mechanics.

To avoid any misunderstandings, let us once more stress the active role of one substance only (e.g., the random medium). In the conventional statistical physics problem of a diffusion of one gas (ink) in another (milk), the Brownian motion of each gas separately comes exclusively from the molecular agitation of its own constituents, based on the assumption of their simultaneous presence in abundance. In our case the random medium can be interpreted conventionally, while the ink (using the analogy) ensemble is constructed by considering the completely independent single-particle-random-medium (joint in our case) propagation problems.

In the configuration-space description of the standard Brownian motion [1,3] the statistical destiny of the particle following a random path $X_t, (X_t \in \mathbb{R}^1, t_1 \leq t \leq t_2)$ is completely determined by the fundamental *microscopic law of random displacements*, i.e., the transition probability density of the diffusion process for small times. Its primordial (Einstein's) version tells us that irrespective of the actual particle position and time spent in contact with the random environment, the effect of random fluctuations remains statistically the same on the chosen time scale Δt . Namely, the probability that a particle originat-

ing from a point x at time t will be found between x and $x + \Delta x$ after time $\Delta t > 0$ is given by the formula

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

which does not depend on the reference point (of particle origin) $X_t = x$ reached by the particle in the course of an unspecified, but quite complicated evolution.

Apparently, such a displacement law basically characterizes the random medium itself and its highest possible level of the statistical homogeneity. The only information about a particle proper (like, e.g., its mass) is contained in the diffusion constant D , which is kept fixed if particles of the same sort are subject to the environment perturbing effect in the series of single particle trials (statistical samples).

If we consider the initial probability distribution of the random variable X_t (representing a particle in the course of the stochastic diffusion process) to be given by

$$\rho_0(x) = (\pi \alpha^2)^{-1/2} \exp \left[-\frac{x^2}{\alpha^2} \right], \quad (2)$$

then its statistical evolution, as a consequence [4,5] of (1), is given by the familiar heat kernel:

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

$s \leq t$,

$$\rho(x, t) = \int \rho(y, s) p(y, s, x, t) dy \\ = [\pi(\alpha^2 + 4Dt)]^{-1/2} \exp \left[-\frac{x^2}{\alpha^2 + 4Dt} \right], \quad (3)$$

$$\partial_t \rho = D \Delta \rho,$$

$$\rho(x, 0) = \rho_0(x),$$

which extends the applicability of the microscopic displacement law (1) to time intervals of arbitrary size.

Let us notice that in addition to the forward transition probability density $p(y, s, x, t)$ allowing for statistical predictions about the future of the diffusing particle, we can as well define a convenient device (actually the backward transition probability density of the process) which makes it possible to reproduce the statistical past of the process, given the present. Indeed, since (3) defines $\rho(x, t)$ for all instants of interest, we can introduce

$$p_*(y, s, x, t) = p(y, s, x, t) \frac{\rho(y, s)}{\rho(x, t)}, \quad s \leq t \quad (4)$$

with the obvious property

$$\int p_*(y, s, x, t) \rho(x, t) dx = \rho(y, s), \quad s \leq t. \quad (5)$$

The transition probability densities $p(y, s, x, t)$ and $p_*(y, s, x, t)$ entail a deeper insight into the microscopic structure of the diffusion process.

For example, the conditional average taken over all po-

sitions starting from which at time $t - \Delta t$ (alternatively) the diffusing particles are given a chance to reach a prescribed point x at time t :

$$E_*^{\Delta t}[x, t] = \int y p_*(y, t - \Delta t, x, t) dy \\ = \left[\int y \rho(y, t - \Delta t) \right. \\ \left. \times p(y, t - \Delta t, x, t) dy \right] / \rho(x, t) \quad (6)$$

in virtue of

$$\int y \rho(y, s) p(y, s, x, t) dy = x \frac{\alpha^2 + 4Ds}{\alpha^2 + 4Dt} \rho(x, t) \quad (7)$$

yields (set $s = t - \Delta t$)

$$E_*^{\Delta t}[x, t] = x - \frac{4Dx}{\alpha^2 + 4Dt} \Delta t = x - b_*(x, t) \Delta t, \quad (8) \\ b_*(x, t) = \frac{4Dx}{\alpha^2 + 4Dt} = -2D \nabla \rho(x, t) / \rho(x, t),$$

where $b_*(x, t)$ plays the role of the mean velocity of (incoming [6] to x at time t) particles, which approach a given point x in the course of the uniform rectilinear motion in a small time interval $[t - \Delta t, t]$. In fact [1], in the absence of external forces the particle should show a certain *tendency* to persist in the uniform rectilinear motion on small time scales Δt . The mean velocity $b_*(x, t)$ denotes here the best possible estimate of such motion tendency *before* x has been reached at time t .

By invoking the standard [1] definition of the backward drift of our diffusion process, we realize that

$$\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \{x - E_*^{\Delta t}[x, t]\} = b_*(x, t) \quad (9)$$

coincides with (8). The analogous best prediction about the *expected* motion tendency in the interval $[t, t + \Delta t]$ comes from

$$E^{\Delta t}[x, t] = \int p(x, t, y, t + \Delta t) y dy = x, \quad (10)$$

which implies

$$\lim_{\Delta t \rightarrow 0} \frac{1}{\Delta t} \{E^{\Delta t}[x, t] - x\} = b(x, t) = 0, \quad (11)$$

hence neither direction is particularly privileged by particles outgoing (originating) from x at time t : there is no specific motion tendency.

Drifts $b_*(x, t)$ and $b(x, t)$ thus give account of a single particle (mean) *tendency* of motion respectively in time intervals $[t - \Delta t, t]$ and $[t, t + \Delta t]$ where x stands for the actual (present) particle location at the time instant t of its random motion [random variable X_t is being propagated by the universal displacement law (1)].

We might wish to analyze the available statistical information *not about a single particle* but about an *ensemble* of particles. In fact, if the initial ($t=0$) random variable X_t (particle) distribution is given by (2), then in virtue of (1) we have immediately initiated the Brownian expansion of the whole ensemble, whose individual constit-

uents execute the previously described Brownian motion scenario. Apparently the random variable (and the ensemble [3]) distribution after time Δt reads

$$\rho_{\Delta t}(x) = [\pi(\alpha^2 + 4D\Delta t)]^{-1/2} \exp \left[-\frac{x^2}{\alpha^2 + 4D\Delta t} \right]. \quad (12)$$

However, if in contrast to the single particle propagation, it is the ensemble evolution which attracts our attention, then a *new* characteristic of motion enters the scene. Namely, we can consistently ask for an average velocity of the locally uniform rectilinear motion on the time scale Δt , which stands for the tendency of motion of a single particle when considered as a member of a particular ensemble. The pertinent analysis was accomplished in Ref. [6] albeit with a slightly different goal in mind, and implies the following: Given the forward drift in the time interval $[t - \Delta t, t]$ (mean velocity of particles outgoing from x at time $t - \Delta t$), $b(x, t - \Delta t)$ and the backward drift $b_*(x, t)$ in the time interval $[t - \Delta t, t]$ (mean velocity of particles incoming to x and time t), then the average velocity of particles propagating (flying) in the vicinity of the point x in the time interval $[t - \Delta t, t]$ reads

$$\frac{1}{2}[b(x, t - \Delta t) + b_*(x, t)] = v_-(x, t), \quad (13)$$

where $v_-(t)$ is the original notation of Ref. [6].

If specialized to our case, we know that $b(x, t) = 0$ for all x and t , while $b_*(x, t)$ is given by the formula (8). In consequence, the mean tendency of motion evaluated for the Brownian ensemble in each time interval Δt preceding a given time instant t is given by

$$v(x, t) = v_-(x, t) = \frac{1}{2}b_*(x, t) = -D\nabla\rho(x, t)/\rho(x, t) \quad (14)$$

in consistency with both the probability conservation law

$$\partial_t \rho = -\nabla(\rho v) \quad (15)$$

and the macroscopic diffusion law [3]

$$\partial_t \rho = D\Delta\rho, \quad (16)$$

which is a direct consequence of the induced particle current $j(x, t) = (\rho v)(x, t)$.

In particular, the average flow implying the Brownian expansion of the $\rho_0(x)$ ensemble to $\rho_{\Delta t}(x)$, (12), is characterized by

$$v(x, \Delta t) = \frac{2Dx}{\alpha^2 + 4D\Delta t} \quad (17)$$

in the time interval $[0, \Delta t]$.

It is interesting to notice that both $\rho(x, t)$ and $(\rho v)(x, t)$ ingredients of the formula (15) come from the propagation of the initial data $\rho_0(x)$ and $(\rho_0 v_0)(x)$, where $v_0(x) = -D\nabla\rho_0/\rho_0$, through the formulas (3) and (7), respectively. The reader must, however, be aware of the fact that although

$$(\rho v)(x, t) = \int p(y, 0, x, t) \rho_0(y) v_0(y) dy \quad (18)$$

holds true, the quantity $v_0(y)$ is *not* an initial average par-

ticle velocity at all, if we refer to the Brownian expansion of the initially static ensemble.

In virtue of (17) the purely Brownian scattering of particles implemented by the displacement law (1), *locally* (in the vicinity of each point x) induces a nontrivial momentum $mv(x, t)$ transfer. Even if the overall averaging $\int v(x, t)\rho(x, t)dx = 0$ does not give any hint, *locally* the momentum cannot be gained from nowhere by independently propagating members of the considered ensemble. If such gain does appear, then by elementary conservation laws (here adopted in the local mean) it *must* arise at the expense of the random environment.

We are quite intentionally using the word ‘‘momentum’’ although a pedestrian understanding of the Einstein diffusion is completely devoid of this notion. By classical arguments [1,3], the configuration-space diffusions (see also Refs. [6-8] need to be derivable from random phase-space motions to be placed on the sound physical basis of the problem of random accelerations. In fact, an explicit reference to a physical intuition about how the Brownian diffusion arises is quite rewarding in this case. Let us literally think about the white noise (idealized description of random accelerations) mechanism leading to highly erratic Brownian paths of the configuration-space Brownian (Wiener) diffusion. We shall cite Nelson [1] here, only slightly paraphrasing his original comment on the classic Kappler’s experiment: ‘‘One has the feeling with [Wiener paths] that one can occasionally see where an exceptionally energetic gas molecule [liquid or other random medium constituent] gives the [monitored particle] a kick. This is not true. Even at the lowest [gas] pressure used, an enormous number of collisions takes place per [time unit], and the irregularities in the [paths] are due to chance fluctuations in the sum of enormous numbers of individually negligible events. It is not correct to think simply that jiggles in the Brownian trajectory are due to kicks from molecules. Brownian motion is unbelievably gentle. Each collision has an entirely negligible effect on the the position of the Brownian particle, and it is only fluctuations in the accumulation of an enormous number of very slight changes in the particle’s velocity which give the trajectory its irregular appearance.’’

However (we are not far away from Boltzmann’s discussion of collisions in the kinetic theory of gases and liquids), even the slightest change in the individual particle velocity is accomplished by locally imparting a concrete amount of momentum to the random environment, if its opposite is imparted to a particle itself. Then only the momentum conservation law in any collision event will not be violated. We should have indeed the action-reaction principle respected in the random accelerations problem.

In our previous discussion, the agitation of particles represented by the law of random displacements (1) was found to induce the nontrivial and non-negligible (macroscopic regime) particle flows, when considered on the ensemble average. Since we are dealing with massive particles, the momentum conservation law tells us that on the ensemble average, the individually negligible momentum losses or gains by the random environment (individual recoils) give rise to the nontrivial and non-negligible *recoil*

effect (local turbulences [9]) in the random medium itself.

The *local Brownian recoil principle* can be formulated as follows: If Brownian fluctuations due to the medium produce an average field of local particle flows $\bar{v}(x, t)$, then an average field of local drifts $-\bar{v}(x, t)$ is induced in

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

$$b(y, t) = -\bar{v}(y, t), \quad (19)$$

$$p_0(y, 0, x, \Delta t) = (4\pi D \Delta t)^{-1/2} \exp \left[-\frac{(x - y)^2}{4D \Delta t} \right].$$

By starting at time $t=0$ from the distribution $\rho_0(x)$, after time Δt we arrive at the new particle distribution $\rho_{\Delta t}(x)$, (12), resulting from the ensemble expansion with the mean velocity field $\bar{v}(x, \Delta t)$, (17). Because of the Brownian recoil principle we have induced turbulences of the random environment, whose ensemble average gives rise to the field of mean drifts (flows in the medium) $b(x, \Delta t) = -\bar{v}(x, \Delta t)$. The universal displacement law (1) for the next period Δt of the random propagation is replaced by the field of local displacement laws $p_{\Delta t}(y, \Delta t, x, 2\Delta t)$ as given by (19). Let us denote

$$\beta^2 = \alpha^2 + 4D \Delta t, \quad \bar{v}(x, \Delta t) = 2Dx / \beta^2, \quad \rho_{\Delta t}(x) = (\pi\beta^2)^{-1/2} \exp(-x^2 / \beta^2) = \rho_\beta(x) \quad (20)$$

and investigate the transition probability density

$$p(y, 0, x, t) = (4\pi Dt)^{-1/2} \exp \left[-\frac{(x - y + 2Dyt / \beta^2)^2}{4Dt} \right], \quad t > 0. \quad (21)$$

In the notation $w_{x_0}(x, t)$, $x_0 \rightarrow y$ this object was utilized in Ref. [8], and we know that

$$\int p(y, 0, x, t) (\pi\beta^2)^{-1/2} \exp(-y^2 / \beta^2) dy = \frac{\beta}{[\pi(\beta^4 + 4D^2 t^2)]^{1/2}} \exp \left[-\frac{x^2 \beta^2}{\beta^4 + 4D^2 t^2} \right] = \rho_\beta(x, t) \quad (22)$$

and [cf. formula (45) in Ref. [8]]

$$\int p(y, 0, x, t) \left[\frac{2Dy}{\beta^2} (\pi\beta^2)^{-1/2} \exp(-y^2 / \beta^2) \right] dy = \frac{2D(\beta^2 - 2Dt)x}{\beta^4 + 4D^2 t^2} \rho_\beta(x, t) = -b_\beta(x, t) \rho_\beta(x, t) \quad (23)$$

in close analogy with (3) and (18). The important observation here is [8] that

$$b_\beta(x, t) = -\frac{2D(\beta^2 - 2Dt)x}{\beta^4 + 4D^2 t^2} \quad (24)$$

coincides with the forward drift of the diffusion process of Nelson's stochastic mechanics associated with the solution of the free Schrödinger equation:

$$i \partial_t \psi(x, t) = -D \Delta \psi(x, t), \quad (25)$$

$$\psi(x, 0) = \rho_\beta^{1/2}(x, 0) = (\pi\beta^2)^{-1/4} \exp(-x^2 / 2\beta^2),$$

where, evidently, $\rho_\beta(x, t) = |\psi(x, t)|^2$ and

$$b_\beta(x, t) = u_\beta(x, t) + v_\beta(x, t),$$

$$u_\beta(x, 0) = -\frac{2Dx}{\beta^2} \rightarrow u_\beta(x, t) = -\frac{2D\beta^2 x}{\beta^4 + 4D^2 t^2}, \quad (26)$$

$$v_\beta(x, 0) = 0 \rightarrow v_\beta(x, t) = \frac{4D^2 x t}{\beta^4 + 4D^2 t^2}.$$

the medium itself: the $-\bar{v}$ local drag of particles does compensate the $m\bar{v}$ local momentum associated with the ensemble of Brownian scattered particles. As a consequence the infinitesimal law of random displacements (for the subsequent time interval Δt) takes the form

The conservation law

$$\partial_t \rho_\beta = -\nabla(\rho_\beta v_\beta) \quad (27)$$

should be compared with the previous (conventional Brownian) probability conservation law (15).

As noticed in Ref. [8], we deal here with a concrete realization of Nelson's acceleration formula $(m/2)(D_+ D_- + D_- D_+) X(t) = 0$ in the form of the momentum balance equation (in the conditional mean)

$$\partial_t v_\beta + v_\beta \nabla v_\beta = -\nabla Q_q, \quad (28)$$

where the "quantum potential" $Q_q \rho(x, t) = -2D^2 \Delta \rho_\beta^{1/2}(x, t) / \rho_\beta^{1/2}(x, t)$ has now a definite statistical origin linked with the Brownian propagation of particle ensembles, which is affected (modified) by the Brownian recoil principle.

Let us add that for times $t \gg \Delta t$ we can everywhere in (20)–(28) neglect the initial (purely Brownian phase of motion) Δt contributions, and replace β^2 by α^2 .

It is also instructive to notice that the conventional

Brownian dynamics (3) is characterized by the momentum balance equation

$$\partial_t v + v \nabla v = -\nabla Q, \quad Q = 2D^2 \Delta \rho^{1/2} / \rho^{1/2}, \quad (29)$$

which is an alternative realization of another Nelson's acceleration formula $(m/2)(D_+ D_+ + D_- D_-)X(t) = 0$ valid for Markovian diffusions; see, e.g., Refs. [7,8,10,11] for more details.

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