Why quantum dynamics can be formulated as a Markov process

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We invert the well-developed strategy of studying dynamics in terms of probability densities and investigate the problem of the most likely microscopic propagation scenario, which is consistent with the given *a priori* (possibly phenomenological) input-output statistics data for the process taking place in a finite-time interval. A solution of this so-called Schrödinger problem is known to provide an adequate probabilistic framework for the measure preserving dynamics which is Markovian. We pay particular attention to the subclass of nonstationary solutions, determined by unitary-wave-packet evolution (Schrödinger wave mechanics). The existence of the pertinent Markovian diffusion is known on general grounds, but no explicit demonstration (through detailed computational arguments) until now was available even in the simplest cases. We give a definitive probabilistic description of the free quantum dynamics as a stochastic process solving Schrödinger's interpolation problem. The Markov diffusion arises as a particular case singled out by a suitable Feynman-Kac semigroup.

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I. THE SCHRÖDINGER BOUNDARY DATA PROBLEM

It is clear that a stochastic process is *any* conceivable evolution which we can analyze in terms of probability. In many branches of physics ranging from essentially deterministic to intrinsically random classical and quantum problems, probability measures do naturally arise. The quantum issue should receive particular attention in connection with the Born statistical postulate, which implies that quantum theory deals with densities of probability measures. However, quite generally the stochastic analysis is disregarded as against the pragmatic viewpoint of deducing as many experimentally verifiable or, rather, falsifiable data as possible, even at the price of manipulating the ill-defined or not defined at all ("safe" bypassing of rather fundamental difficulties) probabilistic quantities. We leave aside the epistemological problem of whether the (quantum) measurement theory belongs to quantum mechanics proper or not, but cannot leave without comment the surprising title phrase [1], hastily elevated to the status of a generally valid statement, "why quantum mechanics cannot be formulated as a Markov process." It leads the unsuspicious reader much too far, if compared with the real value of arguments and specialized assumptions about the probabilistic structure of the particular (quantum) measurement model, with no mention about the fundamental probabilistic input coming from the Born statistical postulate (sometimes called an interpretation, albeit pervading not only the conceptual but, what is of profound importance, the mathematical structure of the theory), and the quantum dynamics proper. Gillespie's discussion [1] pertains to a simple two-level system responding to a time-dependent perturbation in full accord with the Schrödinger picture evolution principles. It is well known [2–4] that a Markovian modeling of quantum two-level system dynamics (Schrödinger-Pauli) is possible: a mathematically rigorous representation of quantum evolution in terms of the dichotomic (jump) Markov process is here a supplement to the more general framework [5]. However, Gillespie's original goal was *not* merely to investigate whether any Markov process can mimic quantum two-level system dynamics. He carries out his analysis under an additional very restrictive assumption [1]: "that quantum system could be mathematically modeled by a conceptually realistic stochastic system that randomly jumps back and forth, but that is at any instant *definitely* in one state or another." Under this "*definitely* in one state or another" restriction, the Markov representation of the quantum motion was found untenable. And this (epistemological input) assumption must be relinquished to allow for Markov representation.

Clearly, the status of the Markov property in quantum physics has been a traditional subject of controversy since the advent of quanta. It is therefore important to have clearly specified what (when and why) can or cannot be formulated as a Markov process in the framework of quantum mechanics. While emphasizing the issue of the traditional Schrödinger picture evolution, we advocate an approach to the problem initiated by Schrödinger himself [6], whose relevance to quantum physics seems to have been perceived in the 1980s [7]. As long as no extra epistemological assumptions are superimposed on the traditional framework of quantum mechanics, the Schrödinger picture dynamics no doubt allows for a Markovian representation [5, 7, 8], including the case of two-level systems [2–4].

The main idea behind what we call the *Schrödinger problem* [6, 9] is an attempt to get an insight (in fact through modeling) into a physical process, unknown in detail, with a finite time of duration, in terms of (random) motions consistent with the prescribed input-output statistics data, i.e., the boundary distributions for repeatable single particle (sample) procedures. Less specifically, we can simply look for a stochastic evolution which interpolates between the boundary probability measures, in particular, for the (invariant) measure

preserving dynamics [8, 10].

Given a dynamical law of motion (for a particle as example), in many cases one can associate with it (compute or approximate the observed frequency data) a probability distribution. The *inverse operation* of deducing the detailed (possibly individual, microscopic) dynamics, which either implies or is consistent with the given probability distribution (and eventually with its own time evolution) at first glance might look hopeless and not to allow for a unique solution, if any at all.

For clarity of discussion, we shall confine our attention to processes whose random variable $X(t), t \geq 0$, takes values on the real line R^1. In the above input-output statistics context, let us invoke a probabilistic problem, originally due to Schrödinger: given two strictly positive (on an open interval) boundary probability distributions $\rho_0(x), \rho_T(x)$ for a process with the time of duration $T \geq 0$, can we uniquely identify the stochastic process interpolating between them? The answer is known to be affirmative, if we assume the interpolating process to be Markovian. In fact, we get then a unique Markov process, which is specified by the probability measure $m(A,B) = \int_A dx \int_B dy\, m(x,y)$ with marginal densities

$$\int dy\, m(x,y) = \rho_0(x), \quad \int dx\, m(x,y) = \rho_T(y), \tag{1}$$

where the functional form of the joint probability density, which is specialized to yield the Markov process as a solution [9], (this formula was derived for the first time by Schrödinger [6] in his own analysis of conditional Brownian motion), reads

$$m(x,y) = \Theta_*(x,0)\, k(x,0,y,T)\, \Theta(y,T). \tag{2}$$

In the above the time interval border is fixed, and the space variables are allowed to vary. Our notation is in conformity with that in the earlier publications [7, 10], where real functions $\Theta_*(x,t), \Theta(y,s)$ and the strictly positive integral kernel $k(s,y,x,t)$ (take a familiar heat kernel as an example) are considered at the boundaries of the time interval $[0,T]$ with no restrictions on the space variables x, y. The main issue at this point is that the two unknown functions $\Theta_*(x,0), \Theta(y,T)$ are to come out as solutions of *the same sign* of the integral identities (1). Provided, we have at our disposal a bounded strictly positive integral kernel $k(x,s,y,t), 0 \leq s < t \leq T$, then $\Theta_*(x,t) = \int k(0,y,x,t)\Theta_*(y,0)dy$ and $\Theta(x,s) = \int k(s,x,y,T)\Theta(y,T)dy$. The sought for interpolation has a probability distribution $\rho(x,t) = (\Theta_*\Theta)(x,t), t \in [0,T]$, to which a subsequent stochastic analysis should apply.

To have a definite Markov solution in hand, we must decide what is the appropriate choice for the dynamical semigroup kernel in the above. Apparently it is the crucial step in the construction of any explicit random propagation consistent with the boundary measure data.

II. MARKOV DIFFUSION RESPECTING THE NATURAL BOUNDARIES

Our present aim is to make a refinement of the original Nelson findings [5] from a novel (Schrödinger problem) perspective. We wish to discuss *diffusive* solutions only, and take for granted that the traditional Fokker-Planck equation sets the rules of the game for the interpolating probability density. Then we look for the corresponding fundamental transport mechanism (law of random displacements) and choose [7, 8] the transition probability density for the Markov diffusion process in the form

$$p(y,s,x,t) = k(y,s,x,t)\, \frac{\Theta(x,t)}{\Theta(y,s)} \tag{3}$$

with $s \leq t$. The strange-looking form of $p(y,s,x,t)$ is not simply an arbitrary guess, but has a deep motivation in the connection we wish to exploit between the transition probability density p of the Markov diffusion and the Feynman-Kac kernel $k(y,s,x,t)$ defining the local mean dynamics of the stochastic process [10]. Notice that for a given probability density $\rho(y,s) = (\Theta\Theta_*)(y,s)$ there holds

$$\begin{aligned}\int p(y,s,x,t)\Theta(y,s)\Theta_*(y,s)dy &= \int k(y,s,x,t)\Theta_*(y,s)dy\Theta(x,t)\\ &= \Theta_*(x,t)\Theta(x,t) = \rho(x,t);\end{aligned}$$

hence a consistent propagation pattern is reproduced. This transition density is required to come out of the forward Kolmogorov equation (e.g., the Fokker-Planck equation) as its fundamental solution [$p \to \delta(x-y)$ as $t \downarrow s$]. For convenience we simplify the whole problem by fixing a diffusion constant $D > 0$ (this choice narrows the allowed framework slightly):

$$\partial_t \rho = D\triangle_x \rho - \nabla_x(b\rho), \tag{4}$$

where $\rho(x,t) = \int p(y,s,x,t)\, \rho(y,s)\, dy$ with $\rho_0(x) = \rho(x,0)$ and the forward drift $b(x,t) = 2D\, \frac{\nabla\Theta}{\Theta}(x,t)$. In addition we demand that the backward (adjoint) diffusion equation is solved weakly by the same transition density (with respect to another pair of variables)

$$\partial_s p = -D\triangle_y p - b\nabla_y p, \tag{5}$$

where $p = p(y,s,x,t)$, $s \leq t$, $b = b(y,s)$. It implies that we deal here with a *unique* diffusion process, whose transition density is a *common* fundamental solution for both the backward and forward Kolmogorov equations.

To understand the role of the integral kernel $k(y,s,x,t)$ in (1)–(5) let us assume that $\Theta(x,t)$ is given in the form (drifts are gradient fields as a consequence) $\Theta(x,t) = \pm\exp\Phi(x,t) \Rightarrow b(x,t) = 2D\nabla\Phi(x,t)$, $x \in (r_1, r_2)$, and insert (3) into the Fokker-Planck equation (4). Then the kernel must be a fundamental solution [$k(y,s,x,t) \to \delta(x-y)$ as $t \downarrow s$] of the generalized diffusion equation for $\theta_*(x,t)$:

$$\partial_t\, \theta_* = D\triangle_x\, \theta_* - \frac{1}{2D}\Omega(x,t)\, \theta_*, \tag{6}$$

$$\Omega(x,t) = 2D\left[\partial_t\Phi + \frac{1}{2}\left(\frac{b^2}{2D} + \nabla b\right)\right],$$

and to guarantee (2) it must display the semigroup composition properties.

Notice that the backward diffusion equation takes the form of the adjoint to (6), now with respect to $\theta(y,s)$:

$$\partial_s \theta = -D\triangle_y \theta + \frac{1}{2D}\Omega(y,s)\,\theta. \tag{7}$$

The diffusion process is then known to be confined between the so-called natural boundaries (they are "naturally," with no external agencies involved, respected by the process), which mathematically correspond to the Dirichlet boundary conditions (vanishing density). If the process takes place in between natural boundaries at infinity, the standard restrictions on the auxiliary potential Ω and hence on the drift potential $\Phi(x,t)$, yield the familiar Feynman-Kac representation of the fundamental solution $k(y,s,x,t)$:

$$\int dy\Theta_*(y,s)k(y,s,x,t)$$
$$= \int dy\Theta_*(y,s)\int \exp\Big[-\frac{1}{2D}\int_s^t \Omega\Big(X(u),u\Big)du\Big]$$
$$\times d\mu[s,y \mid t,x], \tag{8}$$

which integrates $\exp[-(1/2D)\int_s^t \Omega(X(u),u)du]$ weighting factors with respect to the conditional Wiener measure, i.e., along all sample paths of the Wiener process connecting y with x in time $t-s$. More elaborate discussion is necessary, if at least one of the boundary points is *not* at infinity [10].

Let us notice that the time independence of Ω is granted if Φ is either independent of time or depends on time at most linearly. Then, the standard expression $\exp[-H(t-s)](y,x)$ for the kernel k clearly reveals the involved semigroup properties, with $H = -D\triangle + (1/2D)\Omega(x)$ being the essentially self-adjoint operator on its (Hilbert space) domain.

In the previous paper [10] we narrowed the scope of our discussion and analyzed in detail the case of diffusions whose drift fields are time independent, $\partial_t b(x,t) = 0$ for all x, and the process is confined between the natural boundaries, not necessarily at infinity. For our present purpose the assumption that boundaries are natural means that the process cannot reach them in a finite time. Under these circumstances the standard rules of the Itô calculus retain their validity and the diffusion process $X(t)$ "admits the stochastic differential" with respect to the standard Wiener process $W(t)$:

$$dX(t) = b\big(X(t),t\big)dt + \sqrt{2D}dW(t),$$
$$X(0) = x_0\,,\ t \in [0,T], \tag{9}$$

for all times. The weak [in view of assigning the density $\rho_0(x)$ to the random variable $X(0)$] solution of (9) is thus well defined.

An interesting aspect of the (formal) infinitesimal increment formula (9) is that it allows for a derivation of the Fokker-Planck equation. Then, having given $p(y,s,x,t)$ for any smooth function of the random variable, the forward time derivative in the conditional mean can be introduced (we bypass in this way the inherent non-differentiability of sample paths of the process)

$$\lim_{\triangle t\downarrow 0}\frac{1}{\triangle t}\left[\int p(x,t,y,t+\triangle t)f(y,t+\triangle t)dy - f(x,t)\right]$$
$$= (D_+f)(X(t),t)$$
$$= (\partial_t + b\nabla + D\triangle)f(X(t),t), \tag{10}$$

with $(D_+X)(t) = b(x,t)$, $X(t) = x$, so that the second forward derivative associates with our diffusion a local field of accelerations

$$(D_+^2X)(t) = (D_+b)(X(t),t)$$
$$= (\partial_t b + b\nabla b + D\triangle b)(X(t),t)$$
$$= \nabla\Omega(X(t),t) \tag{11}$$

induced by the (auxiliary) potential $\Omega(x,t)$ [(6)]. Since we have given $\rho(x,t)$ for all $t \in [0,T]$, the notion of the backward transition density $p_*(y,s,x,t)$ can be introduced through the identity $\rho(x,t)p_*(y,s,x,t) = p(y,s,x,t)\rho(y,s)$. It allows one to define the backward derivative of the process in the conditional mean,

$$\lim_{\triangle t\downarrow 0}\frac{1}{\triangle t}\left[x - \int p_*(y,t-\triangle t,x,t)ydy\right]$$
$$= (D_-X)(t) = b_*(X(t),t)$$
$$= [b - 2D\nabla\ln\rho](X(t),t)\ , \tag{12}$$

$$(D_-f)(X(t),t) = (\partial_t + b_*\nabla - D\triangle)f(X(t),t).$$

Apparently there holds [11, 12]

$$(D_+^2X)(t) = (D_-^2X)(t) = \partial_t v + v\nabla v + \nabla Q = \nabla\Omega, \tag{13}$$

where

$$v(x,t) = \frac{1}{2}(b+b_*)(x,t),$$
$$u(x,t) = \frac{1}{2}(b-b_*)(x,t) = D\nabla\ln\rho(x,t) \tag{14}$$

and

$$Q(x,t) = 2D^2\,\frac{\triangle\rho^{1/2}}{\rho^{1/2}} \tag{15}$$

has the familiar, albeit unexpected because of the context (not quantum as yet, all this is valid for the conventional Brownian motion and Smoluchowski diffusions [13, 14]), form of the de Broglie–Bohm "quantum potential." Let us notice that by means of (13)–(15) we can transform the Fokker-Planck equation into the continuity equation, so that the diffusion process $X(t)$ induces the manifestly *hydrodynamical* local conservation laws (moment equations in the kinetic theory lore)

$$\partial_t\rho = -\nabla(\rho v),$$
$$\partial_t v + v\nabla v = \nabla(\Omega - Q), \tag{16}$$
$$\rho_0(x) = \rho(x,0)\,,\ v_0(x) = v(x,0),$$

which form a closed (in fact, Cauchy) nonlinearly coupled system of differential equations. It is important to know that these local laws do not specify a diffusion uniquely; they characterize the whole family of formally distinct (but equivalent in terms of local averages) diffusion processes.

In view of the natural boundaries [where the density $\rho(x,t)$ vanishes], the diffusion respects a specific ("Euclidean looking") version of the Ehrenfest theorem [10]:

$$E[\nabla Q]=0 \Rightarrow \frac{d^2}{dt^2}E[X(t)]=\frac{d}{dt}E[v(X(t),t)]$$
$$=E[(\partial_t v+v\nabla v)(X(t,t)]$$
$$=E[\nabla\Omega(X(t),t)]. \tag{17}$$

Remark 1. Notice [12, 10] that the auxiliary potential of the form $\Omega = 2Q - V$, where V is any Rellich class representative while Q is defined by (13), gives rise to Nelson's [5,8] diffusion for which $E[\nabla Q]=0 \Rightarrow E[\nabla\Omega] = -E[\nabla V]$ and the "standard looking" form of the second Newton law in the mean arises, with V playing the role of the external force potential. The dimensional factor $\frac{1}{m}$ is incorporated in the definition of V. Let us add that the formula (17) at first glance might not resemble the original textbook form [15] of the Ehrenfest formula, and the meaning of "Euclidean looking" might seem obscure. It is enough to set $\Omega = 2Q - V$ in (16) to pass to the local conservation laws of Nelson's diffusions, with their apparent hydrodynamical implementation [16]. Then a comparison with formulas (8)–(12) of Ref. [16] shows that an exact quantum mechanical Ehrenfest theorem is in hand, with the right-hand side of (17) equal $-\nabla V$ as opposed to the "Euclidean" (set $t \to it$ in the second derivative with respect to time) ∇V; see, e.g., also Sec. III B of Ref. [7].

III. QUANTUM DYNAMICS AS A MARKOV DIFFUSION PROCESS

A. The microscopic transport mechanism (transition probability density) of the process

Let us now pass to the explicit quantum mechanical considerations with the goal of representing the Schrödinger wave mechanics as an integral part of the theory of Markov diffusion processes. That is, we shall analyze some consequences of the statistical postulate, primordial for quantum theory, albeit frequently underestimated, due to Max Born: the identification of the squared modulus of the Schrödinger wave function with the probability density ("of something if anything," but undoubtedly of a certain probability measure) is what embeds quantum mechanics in the theory of stochastic processes. Basically we are in the premises of Nelson's stochastic mechanics [5], but now a nontrivial amelioration of the original theory is possible thanks to the Schrödinger problem analysis.

Before investigating the major issue of the nonstationary dynamics, let us indicate a specific example of the invariant probability measure and the induced measure preserving stochastic dynamics. Let us consider the Sturm-Liouville problem on $L^2(R^1)$

$$\left(-\frac{1}{2}\triangle_x+\frac{x^2}{2}\right)\phi=-\lambda\phi. \tag{18}$$

The case of $\lambda = \frac{1}{2}$ is a canonical example of the Feynman-Kac integration. Indeed, the integral kernel $[\exp(-Ht)](y,x) = k(y,0,x,t)$ for $H = -\frac{1}{2}\triangle + (\frac{1}{2}x^2 - \frac{1}{2})$ is known to be given by the formula

$$k(y,0,x,t)=\pi^{-1/2}(1-e^{-2t})^{-1/2}$$
$$\times\exp\left[-\frac{x^2-y^2}{2}-\frac{(e^{-t}y-x)^2}{2}\right]. \tag{19}$$

$\left(e^{-Ht}\Theta\right)(x) = \int k(y,0,x,t)\Theta(y)dy$, where the integrability property $\int k(y,0,x,t)\exp[\frac{x^2-y^2}{2}]dy = 1$ is simply a statement pertaining to the transition density $p(y,0,x,t)$ of the homogeneous diffusion process, which preserves the Gaussian distribution $\rho(x) = (\Theta\Theta_*)(x) = \frac{1}{\sqrt{\pi}}\exp(-x^2)$, where $\Theta_* = \Theta = \phi$.

Now we are ready to address the issue of the nonstationary diffusion consistent with the unitarily implemented (quantum mechanical) dynamics of the localized (wave packet type) probability distribution. Let us consider the free evolution problem $i\partial_t\psi = -D\triangle\psi$, where clearly $\psi(x,t) = [\rho^{1/2}\exp(iS)](x,t) = \int dx' G(x-x',t)\psi(x',0)$ and the Green function $G(x-x',t) = (4\pi iDt)^{-1/2}\exp[-(x-x')^2/4iDt]$ is a straightforward "imaginary time" version (we refer to the folklore linked to the problem of analytic continuation in time) of the familiar heat kernel. For an initial choice of $\psi(x,0) = (2\pi\alpha^2)^{-1/4}\exp(-x^2/2\alpha^2)$ the evolved wave packet at time $t > 0$ reads

$$\psi(x,t)=\left(\frac{\alpha^2}{\pi}\right)^{1/4}(\alpha^2+2iDt)^{-1/2}$$
$$\times\exp\left(-\frac{x^2}{2(\alpha^2+2iDt)}\right). \tag{20}$$

By defining $\rho(x,t) = (\bar{\psi}\psi)(x,t)$ and

$$p(y,0,x,t)=(4\pi Dt)^{-1/2}$$
$$\times\exp\left[-\frac{(x-y+2Dty/\alpha^2)^2}{4Dt}\right], \tag{21}$$

we realize that

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

and moreover

$$\int p(y,0,x,t)\left[\frac{2Dy}{\alpha^2}(\pi\alpha^2)^{-1/2}\right]\exp\left[-\frac{y^2}{\alpha^2}\right]dy$$
$$=\frac{2D(\alpha^2-2Dt)x}{\alpha^4+4D^2t^2}\rho(x,t)=-b(x,t)\rho(x,t). \tag{23}$$

Here, evidently $\rho(x,t)$ and $v(x,t)$,

$$v(x,t) = b(x,t) - D\nabla\rho(x,t)/\rho(x,t), \tag{24}$$

solve the local conservation laws (16) with $V = 0$ and $\Omega = 2Q$.

However, it seems instructive to have a detailed computational demonstration that the pertinent dynamics is a well-defined solution of the Schrödinger problem, and that we really deal with a process which is unique. To simplify consideration we shall rescale the variables so that effectively $D = 1$ appears everywhere. Then we consider the evolution associated with the continuous mapping

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

$$= [2\pi(1+t^2)]^{-1/2}\exp\left[-\frac{x^2}{2(1+t^2)}\right]. \tag{25}$$

The immediate observation is that, quite unfortunately, even the knowledge of the interpolation $\rho(x,t), 0 \leq t$ does not specify the underlying process uniquely. There exist inequivalent processes which imply the very same dynamics of the probability density

Remark 2. To exemplify this comment, we shall give another form of the law of random displacements, which affects the interpolation (25). Naively, let us choose $p(y,0,x,t) = (2\pi t^2)^{-1/2}\exp[-\frac{(x-y)^2}{2t^2}]$. Notice that in contrast to (21) the time label appears in the second power in the denominator. By inspection one verifies that $\rho(x,t) = \int p(y,0,x,t)\rho(y,0)dy$ carries out the mapping (25) exactly as the former transition density (21) does.

In the above, we have defined the transition probability density implementing the quantum propagation from the initial time instant 0 till any finite time t. The arguments of [14] suggest that the process is singled out uniquely. However, as yet we have no explicit expression for the fundamental trasport mechanism (this defect plagues all of the diffusion problems in Nelson's stochastic mechanics [11]) for arbitrary times, nor the mathematical argument (solution of the Schrödinger problem) allowing us to distinguish one particular diffusion process among many others consistent with (25) and/or (16).

Our process is definitely inhomogeneous in space-time, so that certainly $p(y,s,x,t), s \leq t$ is very different from what the previously utilized formula (11) might suggest. Let us consider a Fourier transform (a characteristic function) of the probability distribution $\rho(x,t)$ as given by (25):

$$\hat{\rho}(p,t) = \frac{1}{\sqrt{2\pi}}\exp\left[-\frac{(1+t^2)p^2}{2}\right]. \tag{26}$$

By assuming that the time evolution of the characteristic function is realized via the multiplicative decomposition

$$\hat{\rho}(p,t) = \exp[-(t-s)p^2][\hat{L}_{st}\hat{\rho}(p,s)], \tag{27}$$

where the characteristic function of the standard Wiener process appears as a factor, and the operation $\hat{L}_{st}$ is acting as a time-dependent scaling transformation

$$[\hat{L}_{st}\hat{\rho}](p,s) = \hat{\rho}(c(s,t)p,s), \tag{28}$$

we realize that

$$c = c(s,t) = \left[\frac{(1-t)^2+2s}{1+s^2}\right]^{1/2} \tag{29}$$

is an appropriate scale parameter: $\hat{\rho}(p,t) = \exp[-(t-s)p^2]\hat{\rho}(cp,s)$. An immediate consequence is that

$$p(y,s,x,t) = [4\pi(t-s)]^{-1/2}\exp\left[-\frac{(x-cy)^2}{4(t-s)}\right] \tag{30}$$

is a proper candidate for a transition density of the random propagation (25) in the time interval $[s,t]$. One can easily calculate the drift $b(x,t) = -\frac{(1-t)}{1+t^2}x$ by following the standard stochastic recipe (10). Then, by means of (12) we can directly evaluate $b_*(x,t) = x\frac{1+t}{1+t^2}$, which implies that $v(x,t) = \frac{1}{2}(b+b_*)(x,t) = \frac{xt}{1+t^2}$ satisfies $\partial_t\rho = -\nabla(v\rho)$. Moreover, by setting $u(x,t) = (b-v)(x,t) = -\frac{x}{1+t^2}$ we arrive at $\partial_t u = -\nabla(uv)$, which is [5] another form of the momentum balance equation in this case.

So far so good; there is bad news for those who would expect that everything goes smoothly as in the classical probabilistic considerations. Once we have a transition density for arbitrary times, the obvious step would be to check the Chapman-Kolmogorov formula for the case when the Markov property is expected to hold true. There is a surprise (although not that great, since the transition density must [14] depend on the probability distribution $\rho(y,s)$ at the initial propagation time instant s). The almost obvious, seemingly indisputable formula

$$\int p(y,s,z,u)p(z,u,x,t)dz = p(y,s,x,t) \tag{31}$$

where $s \leq u \leq t$, does *not* hold true as a strong identity. Nevertheless, a direct inspection demonstrates that

$$\int dy\,\rho(y,s)p(y,s,x,t)$$

$$= \int dz\rho(z,u)p(z,u,x,t)$$

$$= \int dz \int dy\rho(y,s)p(y,s,z,u)p(z,u,x,t) \tag{32}$$

is satisfied, as it should be. Another slightly surprising observation is that, although the Fokker-Planck equation $\partial_t\rho = \triangle\rho - \nabla(b\rho)$ is satisfied, the transition density itself does *not* obey the (strong) forward Kolmogorov equation of the same functional form $\partial_t p(y,s,x,t) = \triangle_x p(y,s,x,t) - \nabla_x[b(x,t)p(y,s,x,t)]$, as expected if the transition mechanism is the same for all densities (which is a generic property of all classical diffusions).

Remark 3. One may ask at this point whether any Kolmogorov type equation is obeyed by the transition

density $p(y,s,x,t)$ [(30)]. Let us introduce a conditional expectation value for stochastic flows emanating from the point y at the time instant $s<t$:

$$b_t(y,s)=\lim_{\triangle t\downarrow 0}\frac{1}{\triangle t}\int x[p(y,s,x,t+\triangle t)-p(y,s,x,t)]dx$$
$$\longrightarrow b_t(y,s)=y\frac{\partial c(s,t)}{\partial t}.$$

Then, the following Kolmogorov type equation holds true:

$$\partial_t p(y,s,x,t)=\triangle_x p(y,s,x,t)-b_t(y,s)\nabla_x p(y,s,x,t).$$

Notice that $b_t(y,t)=b(y,t)$ as defined before, by means of (21). The process is *not* characterized by (4), (5) and we need to know what the reason is.

B. The uniqueness, or how the Schrödinger problem sets it

As mentioned before, a general defect of Nelson's diffusions is that usually one knows how, on general grounds, to reconstruct them from any (locally single valued) solution of the Schrödinger equation, *except* for any recipe allowing one to deduce the transition probability density, which is to be unique for a considered diffusion. Let us emphasize that it is impossible to set a definitive probabilistic framework encompassing the unitary-wave-packet evolution, without a microscopic transport rule (transition density) in hand.

Let us therefore analyze the issue from the Schrödinger problem perspective. By taking the Madelung decomposition of a complex function $\psi(x,t)=\exp(R+iS)$ where$R(x,t),S(x,t)$ are real, we can introduce the *new* real functions $\theta=\exp(R+S),\theta_*=\exp(R-S)$ such that (cf. a textbook form of the corresponding wave packet)

$$R(x,t)=-\frac{1}{4}\ln 2\pi(1+t^2)-\frac{x^2}{4(1+t^2)},$$
$$S(x,t)=\frac{x^2}{4}\frac{t}{1+t^2}-\frac{1}{2}\arctan t \tag{33}$$

implies

$$\theta(x,t)=[2\pi(1+t^2)]^{-1/4}\exp\left(-\frac{x^2}{4}\frac{1-t}{1+t^2}\right)\times\exp\left(-\frac{1}{2}\arctan t\right),$$
$$\theta_*(x,t)=[2\pi(1+t^2)]^{-1/4}\exp\left(-\frac{x^2}{4}\frac{1+t}{1+t^2}\right)\times\exp\left(\frac{1}{2}\arctan t\right), \tag{34}$$

where, strikingly, there hold [compare, e.g., the formula (6)]

$$\partial\theta=-\triangle\theta+\frac{1}{2}\Omega\theta,$$
$$\partial\theta_*=\triangle\theta_*-\frac{1}{2}\Omega\theta, \tag{35}$$
$$\frac{1}{2}\Omega(x,t)=\frac{x^2}{2(1+t^2)^2}-\frac{1}{1+t^2}=2\frac{\triangle\rho^{1/2}}{\rho^{1/2}}=Q(x,t).$$

Hence $\Omega(x,t)=2Q(x,t)$, as anticipated before in connection with (17). Moreover, the function $k(y,s,x,t)=p(y,s,x,t)\frac{\theta(y,s)}{\theta(x,t)}$ is a propagator associated with the above equations:

$$\theta_*(x,t)=\int k(y,s,x,t)\theta_*(y,s)dy,$$
$$k(y,s,x,t)=[4\pi(t-s)]^{-1/2}\left(\frac{1+t^2}{1+s^2}\right)^{1/4}\exp\frac{1}{2}(\arctan t-\arctan s)\exp\left[-\frac{(x-cy)^2}{4(t-s)}-\frac{y^2}{4}\frac{1-s}{1+s^2}+\frac{x^2}{4}\frac{1-t}{1+t^2}\right], \tag{36}$$

and the functions $\Theta_*(x,0),\Theta(y,T)$ constitute a solution of the Schrödinger problem (1) and (2) set on the time interval $t\in[0,T]$. Although the form of the strictly positive kernel $k(y,s,x,t)$ does not look that promising, it is possible to check through a direct evaluation that the defining properties of the fundamental solution of the generalized diffusion equation, as listed in Ref. [8], are respected (except for the semigroup composition property):

(a) $k(y,s,x,t)$ is continuous in all variables;

(b) the kernel is strictly positive and $k(y,s,x,t)\to 0$ when $\mid x\mid$ goes to ∞;

(c) $\lim_{\triangle s\downarrow 0}\int k(y,s,x,s+\triangle s)dx=1$;

(d) $\lim_{\triangle s\downarrow 0}\frac{1}{\triangle s}\int(x-y)k(y,s,x,s+\triangle s)=0$; and

(e) $\lim_{\triangle s\downarrow 0}\frac{1}{\triangle s}[1-\int k(y,s,x,s+\triangle s)dx]=\frac{1}{2}\Omega(y,s)$.

The property (e) is of particular importance here, since it clearly reveals what dynamical semigroup was implicitly involved in the, seemingly incidental, definition of the transition probability density (30). The proof of (e) is a bit more complicated than that for cases (a)–(d). Therefore we shall give a complete demonstration below.

Proof. The dynamical semigroup induced property (e).

By substituting $t=s+\triangle s$ while evaluating the integral we get

$$I=\int\exp\left[-\frac{(x-cy)^2}{4\triangle s}\right]\exp\left[x^2\frac{1-t}{4(1+t^2)}\right]dx$$
$$=\frac{\sqrt{4\pi}}{a}\exp\left[-\frac{y^2}{4}\left(\frac{c^2}{\triangle s}-\frac{c^2}{a^2(\triangle s)^2}\right)\right], \tag{37}$$
$$a=\left[\frac{1}{\triangle s}-\frac{1-t}{1+t^2}\right]^{1/2}.$$

Consequently,

$$\int k(y,s,x,s+\triangle s)dx = (a^2\triangle s)^{-1/2}\left(\frac{1+t^2}{1+s^2}\right)^{1/4}\exp\left[\frac{1}{2}\left(\arctan t-\arctan s-\frac{y^2}{4}\frac{1-s}{1+s^2}\right)-\frac{y^2}{4}\left(\frac{c^2}{\triangle s}-\frac{c^2}{a^2(\triangle s)^2}\right)\right]. \tag{38}$$

We shall take advantage of the smallness of the time increment $\triangle s$ and expand the above expression up to terms linear in $\triangle s$. For this purpose let us notice that

$$a^2\triangle s = 1-\frac{1-t}{1+t^2}\triangle s \simeq 1-\frac{1-s}{1+s^2}\triangle s \longrightarrow (a^2\triangle s)^{-1/2}\simeq 1+\frac{1-s}{2(1+s^2)}\triangle s,$$

$$\left(\frac{1+t^2}{1+s^2}\right)^{1/4}\simeq 1+\frac{s\triangle s}{2(1+s^2)},$$

$$\exp\frac{1}{2}(\arctan t-\arctan s)\simeq 1+\frac{\triangle s}{2(1+s^2)}. \tag{39}$$

For the third term in the exponent of (38) we have

$$\frac{c^2}{\triangle s}-\frac{c^2}{a^2(\triangle s)^2}=\frac{c^2}{\triangle s}\left(\frac{a^2\triangle s-1}{a^2\triangle s}\right)\simeq\frac{c^2}{\triangle s}\left[\frac{1-t}{1+t^2}\triangle s-\left(\frac{1-t}{1+t^2}\right)^2(\triangle s)^2\right]$$

$$\simeq -\frac{c^2}{\triangle s}\left[\frac{1-s}{1+s^2}\triangle s-\frac{(\triangle s)^2}{1+s^2}-\frac{2s(1-s)}{(1+s^2)^2}(\triangle s)^2+\frac{(1-s)^2}{(1+s^2)^2}(\triangle s)^2\right]. \tag{40}$$

Because of $c^2\simeq 1-\frac{2(1-s)}{1+s^2}\triangle s$ we get

$$\frac{c^2}{\triangle s}\left(1-\frac{1}{a^2\triangle s)}\right)\simeq -\left[\frac{1-s}{1+s^2}-\frac{2\triangle s}{(1+s^2)^2}\right] \tag{41}$$

and, as a consequence,

$$\frac{1-s}{1+s^2}+\frac{c^2}{\triangle s}\left(1-\frac{1}{a^2\triangle s}\right)\simeq\frac{2\triangle s}{(1+s^2)^2}. \tag{42}$$

Finally, after collecting all terms, we arrive at the following result:

$$\int k(y,s,x,s+\triangle s)dx\simeq\left(1+\frac{\triangle s}{2(1+s^2)}\right)\left(1+\frac{1-s}{1+s^2}\frac{\triangle s}{2}\right)\left(1+\frac{s\triangle s}{2(1+s^2)}\right)\left(1-\frac{y^2}{2}\frac{\triangle s}{(1+s^2)^2}\right)$$

$$\simeq\left(1+\frac{\triangle s}{1+s^2}\right)\left(1-\frac{y^2}{2}\frac{\triangle s}{(1+s^2)^2}\right)\simeq 1+\frac{\triangle s}{1+s^2}-\frac{y^2}{2}\frac{\triangle s}{(1+s^2)^2}. \tag{43}$$

Apparently the dynamical-semigroup-implemented identity (e) follows:

$$\lim_{\triangle s\downarrow 0}\frac{1}{\triangle s}\left[1-\int k(y,s,x,s+\triangle s)dx\right]$$

$$=\frac{y^2}{2}\frac{1}{(1+s^2)^2}-\frac{1}{1+s^2}=\frac{1}{2}\Omega(y,s)=Q(y,s), \tag{44}$$

as expected from the fundamental solution of the generalized diffusion equation. but the semigroup composition property *does not* hold true.

Following the formula (17) we made a comment that Nelson's diffusions are related to the Feynman-Kac potential $\Omega=2Q-V$, which is to appear in the expression (8). In our case the evolution is unaffected by external force fields, i.e., we have the external potential vanishing, $V=0$. Hence the time- (through the density-) dependent potential $\Omega=2Q$ is what remains in the Feynman-Kac expression (8) for the dynamical semigroup kernel, associated with the purely probabilistic image of the free unitary-(quantum-) wave-packet evolution, if ruled by (4), (5).

All probabilistic features characteristic for a solution of the Schrödinger problem were thereby recovered, except for the Markov property: our kernel (36) is *not* a semigroup kernel, as it should be to quarantee the validity of (4), (5).

Remark 4. The very formulation of the Schrödinger problem might leave an impression that it is the simultaneous knowledge of the past (initial data) and of the future (terminal data) of the process, nontrivially involved, that yield the diffusion process itself. One should realize that the boundary data intervene, *if and only if*

it is our intention to reconstruct *a posteriori* the most likely (but unique) microscopic propagation scenario consistent with them. For the actual particle dynamics, the uniqueness information is immaterial, and the local conservation laws (16) determine the stochastic process sufficiently to imply a consistent propagation of the local fields $\rho(x,t), v(x,t)$. We can easily formulate a finite-time partitioning recipe for the purely causal implementation of the intrinsically random motion, which propagates forward the given initial data ρ_0, v_0, as follows.

(i) Set $t - s = \triangle s$ to be small; start from the transition density for the time interval $\triangle s$ with the initial distribution $\rho(x,0) = \rho_0(x)$ and an arbitrary initial drift $b_0(x) = b(x,0) = D\nabla \ln[\rho_0(x)] + v_0(x)$, where $v_0(x)$ is an initial local current-velocity field (one can in principle set it equal to 0, but a better idea in the the quantum case is to relate it to ρ_0 via the concept of the Brownian recoil principle [14]). The terminal density (after time $\triangle s$) immediately arises since, by standard arguments, we have explicitly defined the transition density for any small time interval $\triangle s = t - s > 0$ in terms of $\rho(x,s), v(x,s)$:

$$\int \rho(y,s)p(y,s,x,s+\triangle s)\,dy$$

$$= \int \rho(y,s)(4\pi D\triangle s)^{-1/2} \times \exp\left[-\frac{(x-y-b(y,s)\triangle s)^2}{4\pi D\triangle s}\right] dy.$$

(ii) The terminal drift after the propagation time $\triangle s$ can be evaluated by exploiting the finite difference formula coming from (16),

$$b(x,s+\triangle s) = v(x,s+\triangle s) + D\nabla \ln[\rho(x,s+\triangle s)],$$

$$v(x,s+\triangle s) \approx v(x,s) + [-(v\nabla v)(x,s) + \nabla(Q-V)(x,s)]\triangle s.$$

It is to be compared with the analogous formula for the Smoluchowski propagation starting with the very same data [10, 13]: the difference is in the force term, where $-(Q-V) = V - Q$ takes the place of $Q - V$; compare, e.g., (17).

(iii) The new drift $b(x, s+\triangle s)$ is now taken as the initial drift for the *subsequent* time $\triangle s$ propagation. Knowing that the new (after time $\triangle s$) density is $\rho(x, s+\triangle s)$, we take it as an initial density for the subsequent propagation interval as well.

(iv) All consecutive $\triangle s$ propagation steps are supposed to repeat this feedback pattern up to the required terminal time $T = n\triangle s$. The only probabilistic input in here is the knowledge of the small time transition probability density for each time interval and the validity of the Chapman-Kolmogorov formula. Thus the chosen initial data are causally propagated into the *a priori* unknown terminal ones $\rho(x,T), v(x,T)$. Only after associating $\rho_0(x)$ with $\rho(x,T)$ can we attempt to single out a unique Markov process responsible for the *realized* interpolation.

Remark 5. It is instructive to see how the previous point (iv) works for the just considered case of the free quantum dynamics, with $R(x,t), S(x,t)$ given by (33), and the functional form of the kernel $k(y,s,x,t)$ disentangled from the expression for $p(y,s,x,t)$. In fact, we shall produce the more general path integral formula for the transition probability density, which is valid for nonvanishing external potentials as well,

$$\rho(x,t) = \int dy\ \rho(y,s)p(y,s,x,t)$$

$$= \int dy\ \rho(y,s)\ \exp\left[\frac{1}{2}\ln\frac{\rho(x,t)}{\rho(y,s)} + S(x,t) - S(y,s)\right] \lim_{\triangle t \downarrow 0} \int dx_1 \cdots \int dx_n$$

$$\times \left(\prod_{j=1}^{n+1}[4\pi D\triangle t]^{-1/2}\right) \exp\left[-\frac{(x_j - x_{j-1})^2}{4D\triangle t}\right] \exp\left[-\sum_{j=1}^{n}(2Q-V)(x_j,t_j)\frac{\triangle t}{2D}\right].$$

Here $x_0 = y$, $x_{n+1} = x$, and the dimensional factor $\frac{1}{m}$ referring to the mass of the particle is incorporated in the definition of V. One should realize that in the above there appears an exact Radon-Nikodym derivative formula [8,10] relating the probability measure of the (Kato) perturbed Wiener noise with this for the Wiener noise proper: the measures are mutually absolutely continuous. Setting $V = 0$ we recover the free quantum dynamics implemented formula for the unique diffusion process interpolating between $\rho(y,s)$ and $\rho(x,t)$. In particular, one needs $D = 1$ to get a complete notational agreement with our previous discussion. In contrast to (36), the genuine (Feynman-Kac) semigroup kernel is here involved, and the process *is* a Markov diffusion.

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