Natural boundaries for the Smoluchowski equation and affiliated diffusion processes

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The Schrödinger problem of deducing the microscopic dynamics from the input-output statistics data is known to admit a solution in terms of Markov diffusion processes. The uniqueness of the solution is found to be linked to the natural boundaries respected by the underlying random motion. By choosing a reference Smoluchowski diffusion process, we automatically fix the Feynman-Kac potential and the field of local accelerations it induces. We generate the family of affiliated diffusion processes with the same local dynamics but different inaccessible boundaries on finite, semi-infinite, and infinite domains. For each diffusion process a unique Feynman-Kac kernel is obtained by the constrained (Dirichlet boundary data) Wiener path integration. As a by-product of the discussion, we give an overview of the problem of inaccessible boundaries for the diffusion and bring together (sometimes viewed from unexpected angles) results which are little known and dispersed in publications from scarcely communicating areas of mathematics and physics.

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I. THE SCHRÖDINGER PROBLEM: MICROSCOPIC DYNAMICS FROM THE INPUT-OUTPUT STATISTICS

According to Kac and Logan [1], any kind of time development (be it deterministic or essentially probabilistic) that is analyzable in terms of probability deserves the name of the stochastic process. Given a dynamic law of motion (for a particle, for example), in many cases one can associate with it (compute or approximate the observed frequency data) a probability distribution and various mean values. In fact, it is well known that inequivalent finite difference random motion problems may give rise to the same continuous approximant (e.g., the diffusion equation representation of discrete processes). In addition, in the study of nonlinear dynamical systems [2], given almost any (for the purposes of our discussion, basically one-dimensional) probability density, it is possible to construct an infinite number of deterministic finite difference equations whose iterates are chaotic and which give rise to this *a priori* prescribed density.

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), thus cannot have a unique solution. If we disregard the detailed nature (such as its chaotic, jump, random-walk process, phase-space process with friction, etc. implementations) of the given process, it appears [3,4] that the standard Brownian motion and/or the broad class of Markovian diffusion processes incorporating the Wiener noise input provide satisfactory approximations for a large variety of phenomena. It especially pertains to the explicit modeling of any unknown in detail physical process in terms of the input-output statistics (conditional probabilities and averages) of random motions with a finite time of duration.

From now on we shall confine our attention to continuous Markov processes whose random variable $X(t)$, $t \geq 0$, takes values on the real line R^1 and in particular can be restricted (constrained) to remain within the interval $\Lambda \subset R^1$, which may be finite or (semi-)infinite but basically an open set. It boundaries $\partial\Lambda$ (end points) will be denoted r_1, r_2 with $-\infty \leq r_1 < r_2 \leq \infty$.

In the above input-output statistics context, let us invoke a probabilistic problem, originally due to Schrödinger [5–7]: 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? Perhaps unexpectedly in light of our previous comments, the answer is known [6,7] to be affirmative if we assume the interpolating process to be Markovian. In fact, here we get a unique Markovian diffusion, which is specified by the joint probability distribution

$$m(A,B)=\int_A dx \int_B dy\, m(x,y) \;,$$
$$\int dy\, m(x,y)=\rho_0(x) \;, \tag{1}$$
$$\int dx\, m(x,y)=\rho_T(y) \;,$$

where

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

and the two unknown (not necessarily Lebesgue integrable) functions $\Theta_*(x,0), \Theta(y,T)$ 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

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$$\Theta_*(x,t)=\int k(0,y,x,t)\Theta_*(y,0)dy ,$$
$$\Theta(x,s)=\int k(s,x,y,T)\Theta(y,T)dy , \tag{3}$$

and the sought for interpolation has a probability distribution $\rho(x,t)=(\Theta_*\Theta)(x,t)$, $t\in[0,T]$. The transition density

$$p(y,s,x,t)=k(y,s,x,t)\frac{\Theta(x,t)}{\Theta(y,s)} , \tag{4}$$

with $s\le t$, is a fundamental solution [$p\to\delta(x-y)$ as $t\downarrow s$] of the forward Kolmogorov (i.e., Fokker-Planck) equation with a diffusion constant $D>0$ (this choice narrows slightly the allowed framework):

$$\partial_t p = D\Delta_x p - \nabla_x(bp) ,$$
$$\rho(x,t)=\int p(y,s,x,t)\rho(y,s)dy , \tag{5}$$

with $\rho_0(x)=\rho(x,0)$ and the drift $b(x,t)$ given by

$$b(x,t)=2D\frac{\nabla\Theta}{\Theta}(x,t) . \tag{6}$$

The backward diffusion equation is solved by the same transition density

$$\partial_s p = -D\Delta_y p - b\nabla_y p ,$$
$$p=p(y,s,x,t) , \quad s\le t,\ b=b(y,s) . \tag{7}$$

Here we deal 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)–(7) let us assume that $\Theta(x,t)$ is given in the form (drifts are gradient fields as a consequence)

$$\Theta(x,t)=\pm\exp\Phi(x,t)\Longrightarrow b(x,t)=2D\nabla\Phi(x,t) ,$$
$$x\in(r_1,r_2) \tag{9}$$

and insert (4) to the Fokker-Planck equation (5). Then [8–10], if $p(y,s,x,t)$ is to solve (5), the kernel $k(y,s,x,t)$ must be a fundamental solution of the generalized diffusion equation

$$\partial_t k = D\Delta_x k - \frac{1}{2D}\Omega(x,t)k ,$$
$$k(y,s,x,t)\to\delta(x-y) \quad \text{as } t\downarrow s , \tag{10}$$
$$\Omega(x,t)=2D\left[\partial_t\Phi+\frac{1}{2}\left[\frac{b^2}{2D}+\nabla b\right]\right] ,$$

and to guarantee (3) it must display the semigroup composition properties.

Notice that (4) and (9) imply that the backward diffusion equation (7) takes the form of the adjoint to (10):

$$\partial_s k = -D\Delta_y k + \frac{1}{2D}\Omega(y,s)k , \quad k=k(y,s,x,t) . \tag{11}$$

If the process takes place between boundaries at infinity $r_1=-\infty$ and $r_2=+\infty$, the standard restrictions on the auxiliary potential Ω (Rellich class [11,12]), and hence on the drift potential $\Phi(x,t)$, yield the familiar Feynman-Kac representation of the fundamental solution $k(y,s,x,t)$ common for (10) and (11):

$$k(y,s,x,t)=\int \exp\left[-\frac{1}{2D}\int_s^t \Omega(X(u),u)du\right] \times d\mu[s,y\,|\,t,x] , \tag{12}$$

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 which connect y with x in time $t-s$. See, e.g., Refs. [13,14]. More elaborate discussion is necessary if at least one of the boundary points is *not* at infinity.

Let us notice that the time independence of Ω is granted if either Φ is 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 $H=-D\Delta+(1/2D)\Omega(x)$ being the essentially self-adjoint operator on its (Hilbert space) domain.

II. NATURAL BOUNDARIES MAKE DIFFUSION PROCESSES UNIQUE

We shall make one more step towards narrowing slightly the scope of our discussion by admitting diffusion processes (1)–(7) whose drift fields are time independent: $\partial_t b(x,t)=0$ for all x. We know [8] that both the free Brownian motion and the Brownian motion in a field of force in the Smoluchowski approximation belong to this class of processes. We know also [15] that the boundary-value problems for the Smoluchowski equation have a profound physical significance, albeit the attention paid to various cases is definitely unbalanced in the literature. It is then interesting to observe that the situation we encounter in connection with (1)–(7) is very specific from the point of view of Feller's [15–18] classification of one-dimensional diffusions encompassing effects of the boundary data. Our case is precisely the Feller diffusion respecting (confined between) the natural boundaries. An equivalent statement is that boundary points r_1,r_2 are inaccessible barriers for the process, i.e., there is *no* positive probability that any of them can be reached from the interior of (r_1,r_2) within a finite time for all $X(0)=x\in(r_1,r_2)$; see, e.g., Refs. [16,17] and [18], Chap. III.4.

In the mathematical literature [16,17,14] a clear distinction is made between the backward and forward Kolmogorov equations. The backward one defines the transition density of the process, while the forward (Fokker-Planck) one determines the probability distribution (density) of diffusion. With a given backward equation one can usually associate the whole family of forward (Fokker-Planck) equations whose explicit form reflects the particular choice of boundary data. This fundamental distinction seemingly evaporates in our previous discussion (1)–(11), but it is by no means incidental. In fact, according to Feller [16], in order that there exists one and only one [homogeneous, $p(y,s,x,t)=p(t-s;y,x)$] process satisfying $-\partial_t u = D\Delta u + b\nabla u$ in a finite or infinite interval $r_1 < x < r_2$, it is necessary and sufficient that both boundaries are inaccessible (the probability of reaching either of them within a finite time interval must be zero).

A general feature of the inaccessible boundary problems is that the density of diffusion vanishes [15,19] at the boundaries $\rho(r_1)=0=\rho(r_2)$. This property is shared with absorbing barrier processes, which are more familiar in the realm of the statistical physics. The link is indeed very close [16]: conventionally the absorbing barrier process is defined on the closed interval $[R_1,R_2]$; however, we can always consider it on the open set (R_1,R_2). Theorem 7 of Ref. [16] states that, if the boundaries $r_1 < R_1 < R_2 < r_2$ are inaccessible for the process, then transition densities of the absorbing barrier process on (R_1,R_2) as $R_1 \to r_1$, $R_2 \to r_2$ converge to the unique transition density of the diffusion with unattainable boundaries on (r_1,r_2). It implies that locally, the inaccessible boundary problem in principle can be modeled (approximated) to an arbitrary degree of accuracy by the absorbing barrier process.

It is interesting to notice that the classification of Feller's boundaries in the homogeneous case [time-independent drifts, continuous but not necessarily bounded in the interval (r_1,r_2)] follows from investigating the Lebesgue integrability of the Hille functions (see Refs. [15,17,19] for more details):

$$\begin{aligned} L_1(x) &= \exp\left[-\frac{1}{D}\int_{x_0}^{x} b(y)dy\right] \\ &= \exp\{-2[\Phi(x)-\Phi(x_0)]\} , \\ L_2(x) &= L_1(x)\int_{x_0}^{x}\frac{dz}{L_1(z)} \\ &= \exp[-2\Phi(x)]\int_{x_0}^{x}\exp[2\Phi(z)]dz , \end{aligned} \tag{13}$$

where $x \in (r_1,r_2)$ and we have used (9) in (13). Apparently the $\Phi(x_0)$ contribution in $L_1(x)$ is irrelevant and the integrability of $\exp[\pm\Phi(x)]$ matters here.

If $L_1(x)$ is *not* Lebesgue integrable on $[x_0,R]$, where $R=r_1$ or r_2, then R stands for the natural repulsive boundary of the diffusion. If $L_1(x)$ is integrable but $L_2(x)$ is not, then R is a natural attractive boundary for the process, both being inaccessible. As indicated in Ref. [15], there is no universally established terminology and a certain discrimination between Feller's and the Gihman-Skorohod definition is possible, albeit without consequences for our discussion.

Following Ref. [18] let us denote $P_x[\tau_R < \infty]$ the probability that a process originating from $x \in (r_1,r_2)$ would hit the point R at the moment τ_R for the first time. Then, the inaccessibility of boundaries can be expressed by the statements

$$P_x[\tau_R < \infty]=0 , \quad \forall x < R$$

$$P_x[\tau_R < \infty]=0 , \quad \forall x > R$$

for the right and left boundaries, respectively. For the natural boundary, R is inaccessible from the interior of (r_1,r_2) and the interior of (r_1,r_2) is inaccessible from R.

Following this terminology (i) an inaccessible boundary is called attractive if for any $\epsilon>0$ there exists $\delta>0$ such that $P_x[\lim_{t\to\infty}X(t)=R]>1-\epsilon$ for all $x\in(R,R+\delta)$ in case of the left and $x\in(R-\delta,R)$ in case of the right boundary and (ii) an inaccessible (left) boundary is called repelling if for any $x>R$ and $y<x$ we have $P_y[\tau_x < \infty]=1$.

Remark 1. The standard (unrestricted) Brownian motion on R^1 is the most obvious example of diffusion with natural boundaries. It is not quite trivial to construct explicit examples if one of the boundaries is not at infinity. The classic example of diffusion on the half-line with natural boundaries at 0 and $+\infty$ is provided by the so-called Bessel process [17,20], with the diffusion (backward) generator $L_a=\Delta_x+(1+2a)/x\nabla_x$ (we absorb the diffusion constant D in the rescaled time parameter). The point $r_1=0$ is never reached with probability one if $a\geq 0$. In the case of $a=0$ the transition density reads [20]

$$p(t;x_0,x)=\text{const}\times\frac{x}{2t}\exp\left[\frac{-(x^2+x_0^2)}{4t}\right]I_0\left[\frac{xx_0}{2t}\right] , \tag{14}$$

where the modified Bessel function (Ref. [21], Chap. 7) is given by $I_0(\alpha)=\sum_{j=0}^{\infty}\alpha^{2j}/[2^{2j}(j!)^2]$. Another (less explicit, as given in the form of estimates for the transition density) example pertains [22] to the diffusion equation with the one-dimensional harmonic oscillator potential on the half-line $x\geq a>0$. The related constrained path integrals are considered in Refs. [23,24].

As mentioned before, diffusions with inaccessible barriers might have drifts which are unbounded on (r_1,r_2). Hence our discussion definitely falls into the framework of diffusion processes with singular drift fields [25,26]; see also Refs. [27–32], which are *not* covered by standard monographs on stochastic processes. Particularly illuminating in this respect is the analysis of Ref. [25], where for quite general diffusions, the unattainability of nodal sets (on which the probability density vanishes) in a finite time was demonstrated in the sense that $P_x[\tau_R=\infty]=1$. This crucial property (valid for diffusions with natural boundaries as well) allows us to extend the theory of stochastic differential equations and integrals to diffusions whose drifts produce a bad (unboundedness or divergence to infinity) behavior when approaching the boundaries.

We skip the standard details concerning the probability space, filtration, and the process adapted to this filtration (see, however, Refs. [21,33,34]) and notice that a continuous random process $X(t), t\in[0,T]$ with a probability measure P is called a process of the diffusion type if its drift $b(x)$ obeys

$$P\left[\int_0^T |b(X(t))|dt < \infty\right]=1 , \tag{15}$$

and, given the standard Wiener process (Brownian motion) $W(t)$, the integral identity (D constant and positive)

$$X(t)=\int_0^t b(X(s))ds+\sqrt{2D}\,W(t) \tag{16}$$

holds true for the measure P almost surely, although mathematically the original phrase is unambiguous. It means that $W(t)=(1/\sqrt{2D}\,[X(t)-\int_0^t b(X(s))ds]$ is a standard Wiener process with respect to the probability measure P of the process $X(t)$.

For diffusion processes with natural boundaries, we remain within the regularity interval of $b(X(t))$ for all (finite) times, and (15) apparently is valid. Therefore the standard rules of the stochastic Itô calculus [19] can be adopted to relate the Fokker-Planck equation (7) with the natural boundaries to the diffusion process $X(t)$, which [34] "admits the stochastic differential"

$$dX(t)=b(X(t))dt+\sqrt{2D}\,dW(t)\;,\qquad X(0)=x_0, t\in[0,T] \tag{17}$$

for all (finite) times. The weak [in view of assigning the density $\rho_0(x)$ to the random variable $X(0)$] solution of (17) is thus well defined.

For stochastic differential equations of the form (17), the explicit Wiener noise input, because of (9), implies that, irrespective of whether natural boundaries are at infinity or not, the Cameron-Martin-Girsanov [35–37] method of measure substitutions which parallel transformations of drifts is applicable. Even though the drifts are generally unbounded on (r_1,r_2), the original theory [35–37] is essentially based on the boundedness demand. It is basically due to the fact that the probabilistic Cameron-Martin formula relating the probability measure P_X of $X(t)$ with the Wiener measure P_W (strictly speaking it is the Radon-Nikodym derivative of one measure with respect to another) reduces to the familiar Feynman-Kac formula [10,14,8,29,38] (with the multiplicative normalization). The problem of the existence of the Radon-Nikodym derivative (and this of the absolute continuity of P_X with respect to P_W, which implies that sets of P_W equal to zero are of P_X equal to zero as well) is then replaced by the standard functional analytic problem [11,12] of representing the semigroup operator kernel via the Feynman-Kac integral with respect to the conditional Wiener measure.

The Feynman-Kac formula is casually viewed to encompass the unrestricted (the whole of R^n) motions; however, it is known to be *localizable* and its validity extends also to finite and semi-infinite subsets of R^1 (R^n more generally), as demonstrated in the context of the statistical mechanics of continuous quantum systems [12,22,39–43]. More specifically, it refers to the Dirichlet boundary conditions for self-adjoint Hamiltonians, which ensure their essential self-adjointness (to yield the Trotter formula).

Remark 2. It is perhaps worthwhile to say a few words about the situation when the process in principle can reach or cross the boundary (nodal surface of the probability density in higher dimensions) in a finite time. As before we limit our discussion to the stationary Markov diffusion process and assume that the drift b is a gradient $\sim\nabla\rho/\rho$. If $\rho=\exp\Phi$, where $\rho^{1/2}$ is *not* an element of the Sobolev space $H^1_{\rm loc}(R^d)$ (i.e., is not integrable on bounded sets, with its first derivative), then it is known [44] that the process can reach or cross the set $N_+=[x\in R^d|\rho=0]$. It is possible [45] to formulate a useful criterion (easy to generalize to higher dimensions) for a "tunneling" (transmission) through a chosen point in R^1; let it be the origin $x=0$. Let us take $b\sim\nabla\Theta/\Theta$. The dynamics is given by the energy form on $L^2(R,dx)$, i.e., $E[f_1,f_2)=\int\nabla f_1\nabla f_2\rho(x)dx$, where obviously $\rho=\Theta\Theta_*=\Theta^2$; compare, e.g., (1)–(7). If $\rho(x)\le A|x|$ in the close vicinity of the origin, at least on one side, then there is *no* tunneling through $x=0$. The process cannot cross this point, but may be absorbed or reflected. One needs a bit stronger restriction to prevent the diffusion from hitting the node: nontransmission and nonhitting are not equivalent concepts, although there is no communication between diffusions on the positive and negative semiaxes, respectively. On the other hand, if $\rho(x)\ge A|x|^\alpha$ with $0<\alpha<1$ in a neighborhood of the origin, then there is a particle transmission (tunneling) through $x=0$. As observed in Ref. [45], according to Feller's classification of boundaries, 0 stands for the regular boundary in this case.

III. HYDRODYNAMIC REPRESENTATION: LOCAL CONSERVATION LAWS AND THE NEWTONIAN DYNAMICS IN MEAN

Let us emphasize the importance of (17) and of the Itô differential formula induced by (17) for smooth functions of the random variable $X(t)$. Its *first* consequence is that, 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 [4,7,19,26] (we bypass in this way the inherent nondifferentiability of sample paths of the process)

$$\lim_{\Delta t\downarrow 0}\frac{1}{\Delta t}\left[\int p(x,t,y,t+\Delta t)f(y,t+\Delta t)dy-f(x,t)\right]=(D_+f)(X(t),t)=(\partial_t+b\nabla+D\Delta)f(X(t),t)\;,\qquad X(t)=x \tag{18}$$

so that the second forward derivative associates with our diffusion the local field of accelerations:

$$(D_+^2X)(t)=(D_+b)(X(t),t)=(\partial_t b+b\nabla b+D\Delta b)(X(t),t)=\nabla\Omega(X(t),t) \tag{19}$$

with the auxiliary potential $\Omega(x,t)$ introduced before in the formula (10). 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 as well

$$\rho(x,t)p_*(y,s,x,t)=p(y,s,x,t)\rho(y,s)\;, \tag{20}$$

which allows to define the backward derivative of the process in the conditional mean (cf. Refs. [8,46–48] for a discussion of these concepts in the case of the most traditional Brownian motion)

$$\lim_{\Delta t\downarrow 0}\frac{1}{\Delta t}\left[x-\int p_*(y,t-\Delta t,x,t)y\,dy\right]$$
$$=(D_-X)(t)=b_*(X(t),t)$$
$$=[b-2D\nabla\ln\rho](X(t),t)\ ,\qquad (21)$$
$$(D_-f)(X(t),t)=(\partial_t+b_*\nabla-D\Delta)f(X(t),t)\ .$$

Apparently, the validity of (19) (cf. Refs. [7,10,26] for related considerations) extends to $(D^2_-X)(t)$ as well

$$(D^2_+X)(t)=(D^2_-X)(t)=\partial_t v+v\nabla v+\nabla Q=\nabla\Omega\ ,$$
$$v(x,t)=\frac{1}{2}(b+b_*)(x,t),\ u(x,t)$$
$$=\frac{1}{2}(b-b_*)(x,t)=D\nabla\ln\rho(x,t)\ ,\qquad (22)$$
$$Q(x,t)=2D^2\frac{\Delta\rho^{1/2}}{\rho^{1/2}}\ .$$

Clearly, if b and ρ are time independent, then (22) reduces to the identity

$$v\nabla v=\nabla(\Omega-Q)\ ,\qquad (23)$$

while in case of constant (or vanishing) current velocity v, the acceleration formula (22) reduces to

$$0=\nabla(\Omega-Q)\ ,\qquad (24)$$

which establishes a very restrictive relationship [49,44,50–52] between the auxiliary potential $\Omega(x)$ [and hence the drift $b(x)$] and the probability distribution $\rho(x)$ of the stationary diffusion. The pertinent random motions have their place in the mathematically oriented literature [49,44,50–53].

Let us notice that (22) allows us to transform the Fokker-Planck equation (7) into the familiar continuity equation, so that the diffusion process $X(t)$ admits a recasting in terms of the manifestly hydrodynamical local conservation laws (we adopt here the kinetic theory lore)

$$\partial_t\rho=-\nabla(\rho v)\ ,$$
$$\partial_t v+v\nabla v=\nabla(\Omega-Q)\ ,\qquad (25)$$
$$\rho_0(x)=\rho(x,0),\quad v_0(x)=v(x,0)\ ,$$

which form a closed (in fact, Cauchy) nonlinearly coupled system of differential equations, strictly equivalent to (7) and (19).

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]:

$$E[\nabla Q]=0\Longrightarrow\frac{d^2}{dt^2}E[X(t)]$$
$$=\frac{d}{dt}E[v(X(t),t)]$$
$$=E[(\partial_t v+v\nabla v)(X(t,t))]=E[\nabla\Omega(X(t),t)]\ .\qquad (26)$$

Notice that the auxiliary potential of the form $\Omega=2Q-V$, where V is any Rellich class representative, defines drifts of Nelson's diffusion processes [10,48] for which $E[\nabla Q]=0\Longrightarrow E[\nabla\Omega]=-E[\nabla V]$, i.e., the "standard looking" form of the second Newton law in the mean arises.

At this point it seems instructive to comment on the essentially hydrodynamical features (compressible fluid or gas case) of the problem (25), where the "pressure" term ∇Q is quite disturbing from the traditional kinetic theory perspective [54,55]. Although (25) has a conspicuous Euler form, one should notice that if the starting point of our discussion would be a typical Smoluchowski diffusion [8] (7) and (17) whose drift is given by the Stokes formula (i.e., is proportional to the external force $F=-\nabla V$ acting on diffusing molecules), then its external force factor is precisely the one retained from the original Kramers phase-space formulation [3,4,15] of the high friction affected random motion. In the Euler description of fluids and gases, the very same force which is present in the Kramers (or Boltzmann in the traditional discussion) equation should reappear on the right-hand side of the local conservation law (momentum balance formula) (25). Except for the harmonic oscillator example, in view of (10) it is generally not the case in application to diffusion processes.

Following the hydrodynamic tradition let us analyze the issue in more detail. We consider a reference volume (control interval) $[\alpha,\beta]$ in R^1 (or $\Lambda\subset R^1$), which at time $t\in[0,T]$ comprises a certain fraction of particles (fluid constituents), for an instant of course. Since we might deal with a flow [proportional to the current velocity $v(x,t)$, (22)] the time rate of particles loss by the volume $[\alpha,\beta]$ at time t is equal to the flow outgoing through the boundaries, i.e.,

$$-\partial_t\int_\alpha^\beta\rho(x,t)dx=\rho(\beta,t)v(\beta,t)-\rho(\alpha,t)v(\alpha,t)\ ,\qquad (27)$$

which is a consequence of the continuity equation. To analyze the momentum balance, let us allow [56] for an infinitesimal deformation of the boundaries of $[\alpha,\beta]$ to have entirely compensated the mass (particle) loss (27)

$$[\alpha,\beta]\to[\alpha+v(\alpha,t)\Delta t,\beta+v(\beta,t)\Delta t]\ .$$

Effectively, we pass then to the locally comoving frame. It implies

$$\lim_{\Delta t\downarrow 0}\frac{1}{\Delta t}\left[\int_{\alpha+v_\alpha\Delta t}^{\beta+v_\beta\Delta t}\rho(x,t+\Delta t)dx-\int_\alpha^\beta\rho(x,t)dx\right]$$
$$=\lim_{\Delta t\downarrow 0}\frac{1}{\Delta t}\left[\int_{\alpha+v_\alpha\Delta t}^{\alpha}\rho(x,t)dx+\Delta t\int_\alpha^\beta(\partial_t\rho)dx\right.$$
$$\left.+\int_\beta^{\beta+v_\beta\Delta t}\rho(x,t)dx\right]=0\ .\qquad (28)$$

Let us investigate what happens to the local flows $(\rho v)(x,t)$ if we proceed in the same way (only leading terms are retained):

$$\int_{\alpha+v_\alpha\Delta t}^{\beta+v_\beta\Delta t}(\rho v)(x,t+\Delta t)dx - \int_\alpha^\beta(\rho v)(x,t)dt$$
$$\sim -(\rho v^2)(\alpha,t)\Delta t + (\rho v^2)(\beta,t)\Delta t + \Delta t\int_\alpha^\beta[\partial_t(\rho v)]dx \ . \quad (29)$$

Because of (25) we have

$$\partial_t(\rho v) = -\nabla(\rho v^2) + \rho\nabla(\Omega - Q) \quad (30)$$

and the rate of change of momentum associated with the control volume $[\alpha,\beta]$ is

$$\lim_{\Delta t\downarrow 0}\frac{1}{\Delta t}\left[\int_{\alpha+v_\alpha\Delta t}^{\beta+v_\beta\Delta t}(\rho v)(x,t+\Delta t) - \int_\alpha^\beta(\rho v)(x,t)\right] = \int_\alpha^\beta \rho\nabla(\Omega - Q)dx \ . \quad (31)$$

However [46],

$$\nabla Q = \frac{\nabla P}{\rho}\ , \quad P = D^2\rho\Delta\ln\rho\ , \quad (32)$$

and consequently

$$\int_\alpha^\beta \rho\nabla(\Omega - Q)dx = \int_\alpha^\beta \rho\nabla\Omega dx - \int_\alpha^\beta \nabla P dx = E[\nabla\Omega]_\alpha^\beta + P(\alpha,t) - P(\beta,t) \ . \quad (33)$$

Clearly, $\nabla\Omega$ refers to the Euler-type volume force, while ∇Q (or more correctly P) refers to the pressure effects entirely due to the particle transfer rate through the boundaries of the considered volume. The latter property can be consistently attributed to the Wiener noise proper: it sends particles away from the areas of larger concentration. See, e.g., Refs. [10,46–48] for a discussion of the Brownian recoil principle, which reverses the original Wiener flows.

As it appears, the validity of the stochastic differential representation (17) of the diffusion (5) implies the validity of the hydrodynamical representation (25) of the process. It in turn gives a distinguished status to the auxiliary potential $\Omega(x,t)$ of (10)–(12). We encounter here [8,10] a fundamental problem of what is to be interpreted by a physicist (observer) as the external force field manifestation in the diffusion process. Should it be dictated by the drift form [3,4,15,57] following Smoluchowski and Kramers or rather by $\nabla\Omega$ entering the evident (albeit "Euclidean looking") second Newton law, respected by the diffusion? In the standard derivations of the Smoluchowski equation, the deterministic part (force and friction terms) of the Langevin equation is postulated. However, what if the experimental data pertain to the local conservation laws such as (25) and (27) and there is no direct (experimental) access to the microscopic dynamics?

If the field of accelerations $\nabla\Omega$ is taken as the primary defining characteristics of diffusion we deal with, then we face the problem of deducing all drifts and hence diffusion processes, which give rise to the same acceleration field and thus form a class of dynamically equivalent diffusion processes.

IV. FEYNMAN-KAC KERNELS ON FINITE AND SEMI-INFINITE DOMAINS WITH INACCESSIBLE BOUNDARIES: DYNAMICALLY EQUIVALENT DIFFUSION PROCESSES

Let us analyze the second consequence of the unattainability of the boundaries, which via (15) gives rise to (17). On the same footing as in the case of (15), we have satisfied another probabilistic identity:

$$P\left[\int_0^T b^2(X(t))dt < \infty\right] = 1 \ . \quad (34)$$

For a diffusion process $X(t)$ with the differential (17), Theorem 6 of Ref. [34] states that (34) is a sufficient and necessary condition for the absolute continuity of the measure $P=P_X$ with respect to the Wiener measure P_W. Since, for any (Borel) set A, $P_W(A)=0$ implies $P_X(A)=0$, the Radon-Nikodym theorem applies [33] and densities of these measures can be related. It is worthwhile to mention the demonstration due to Fukushima [44] that the mutual absolute continuity (the previous implication can be reversed) holds true for most measures we are interested in.

In the notation (12), the conditional Wiener measure $d\mu[s,y|t,x]$ gives rise to the familiar heat kernel if we set $\Omega=0$ identically. It in turn induces the Wiener measure P_W of the set of all sample paths, which originate from y at times s and terminate (can be located) in the Borel set A after time $t-s$:

$$P_W[A] = \int_A dx\int d\mu[s,y|t,x] = \int_A d\mu \ , \quad (35)$$

where, for simplicity of notation, the $(y,t-s)$ labels are omitted and $\int d\mu[s,y|t,x]$ stands for the standard [12] path-integral expression for the heat kernel.

Having defined an Itô diffusion $X(t)$, (5) and (17), with the natural boundaries, we are interested in the analogous [with respect to (35)] path measure P_X,

$$P_X[A] = \int_A dx\int d\mu_X[s,y|t,x] = \int_A d\mu_X \ . \quad (36)$$

The absolute continuity $P_X \ll P_W$ implies the existence of the strictly positive Radon-Nikodym density, which we give in the Cameron-Martin-Girsanov form [33,34]

$$\frac{d\mu_X}{d\mu}[s,y|t,x] = \exp\left[\int_s^t \frac{1}{2D}b(X(u))dX(u) - \frac{1}{2}\int_s^t\frac{1}{2D}[b(X(u))]^2du\right] \ . \quad (37)$$

Notice that the standard normalization appears if we set $D=1/2$, which implies $D\Delta\rightarrow\frac{1}{2}\Delta$ in the Fokker-Planck equation. On account of our demand (9) and the Itô formula for $\Phi(X(t),t)$ we have

$$\frac{1}{2D}\int_s^t b(X(t))dX(t) = \Phi(X(t),t) - \Phi(X(s),s) - \int_s^t du[\partial_t\Phi + \tfrac{1}{2}\nabla b](X(u),u) \quad (38)$$

so that apparently

$$\frac{d\mu_X}{d\mu}[s,y|t,x]=\exp[\Phi(X(t),t)-\Phi(X(s),s)] \times\exp\left[-\frac{1}{2D}\int_s^t\Omega(X(u),u)du\right], \quad (39)$$

with $\Omega=2D\partial_t\Phi+D\nabla b+(1/2)b^2$ introduced before in (10) by means of the substitution of (4) in the Fokker-Planck equation.

In the case of natural boundaries at infinity, the connection with the Feynman-Kac formula (12) is obvious, and we have

$$P_X[A]=\int_A\frac{d\mu_X}{d\mu}d\mu =\int_A dx\int\frac{d\mu_X}{d\mu}[s,y|t,x]d\mu[s,y|t,x], \quad (40)$$

where the second integral refers to the path integration of the Radon-Nikodym density with respect to the conditional Wiener measure; see, e.g., Refs. [10,14,49,44,50–53,58]. In the context of (40) and (12) we can safely assert that the pertinent processes [$X(t)$ and $W(t)$] have coinciding sets of sample paths. The stochastic process "realizes" them merely (via sampling) with a probability distribution (frequency) different from this for the Wiener process $W(t)$.

The situation drastically changes if we wish to exploit the "likelihood ratio" formulas (37) and (39) for diffusion processes confined between the unattainable (natural) boundaries, at least one of which is *not* at infinity. In view of the absolute continuity of P_X with respect to P_W, we must be able to select a subset of Wiener paths which coincide with these admitted by the process $X(t)$, except on sets of measure zero (both with respect to P_X and P_W).

We face here a nontrivial problem of the existence of integral kernels for (Schrödinger) semigroup operators on a bounded or semibounded domain. The constrained version of the formulas (40) and (12) should then integrate over a restricted set of Wiener paths: some of them must be totally excluded and some must "avoid" certain areas (Wiener exclusion of Ref. [41]). This problem was solved in the context of the quantum statistical mechanics [39–42,12] where the Dirichlet boundary data for self-adjoint Hamiltonian are casually associated with the completely absorptive boundaries (cf. also Refs. [29–32,38]). The reason is clear if one leads priority to the Brownian motion proper since there is no natural way for the standard Brownian motion (Wiener process) to prohibit it from reaching or passing any conceivable boundary, except for stopping the process when it is going to happen.

The most transparent way towards the localized Feynman-Kac representation of the Dirichlet (Schrödinger) semigroup on the (originally [38] bounded) domain Λ is by introducing the first exit time T_Λ for the Brownian path started inside Λ (a concrete sample path is labeled by ω):

$$T_\Lambda(\omega)=\inf[t>0;X_t(\omega)\in\Lambda]. \quad (41)$$

Then the integral kernel of the (essentially self-adjoint on Λ, with the Dirichlet boundary data) Hamiltonian $H_\Lambda=(-D\Delta+(1/2D)\Omega)_\Lambda$ is to be given by the conditional expectation

$$\exp(-tH_\Lambda)(s,y,t,x) =E_{y,t-s}\left\{\exp\left[-\int_s^t\Omega(X_u)du\right];t<T_\Lambda|X_t=X(t)=x\right\}, \quad (42)$$

which is an integration (40) restricted to these Brownian paths which, while originating from $y\in\Lambda$ at times s, are conditioned to reach $x\in\Lambda$ at time t, without crossing (but possibly touching) the boundary $\partial\Lambda$ of Λ.

Another way to write down (42) is possible if we define a function $\alpha_\Lambda(\omega)$ on the event set (event=sample path):

$$\alpha_\Lambda=\begin{cases}1 & \text{if } X_t(\omega)\in\Lambda \text{ for all } t\in[0,T]\\ 0 & \text{otherwise}.\end{cases} \quad (43)$$

Here α_Λ is measurable with respect to the conditional Wiener measure and then, e.g., (35) can be replaced by the constrained path integral [22,39–42]:

$$P_\Lambda[A]=\int_A dx\int\alpha_\Lambda(\omega)d\mu_\omega[s,y|t,x]=\int_A d\mu_\Lambda, \quad (44)$$

where $A\subset\Lambda$ and ω is the sample path label [omitted in (35) to simplify notation].

The analysis [22,39,40] of special sets of Wiener measure zero is quite illuminating at this point. Namely, the integral (44) in addition to paths which are strictly interior to Λ admits also paths which *do* touch the boundary $\partial\Lambda$ of Λ for at least one instant $t\in[0,T]$. Fortunately [22,39,40], the P_Λ measure of the set of such (unwanted) trajectories is equal to zero.

Let us now consider a diffusion process $X(t)$, which exists in Λ and for which $\partial\Lambda$ is a natural boundary. Obviously *no* sample path of $X(t)$ can reach (touch) $\partial\Lambda$ in a finite time. By the absolute continuity $P_X \ll P_W$ argument, we know that sets of P_W measure zero are the P_X measure zero sets as well. Hence (44) implies an apparent modification of (36):

$$P_X[A]=\int_A dx\int\alpha_\Lambda(\omega)\frac{d\mu_X}{d\mu}[s,y|t,x]d\mu_\omega[s,y,t,x] \quad (45)$$

applicable to the diffusion $X(t)$ with the natural boundary $\partial\Lambda$. The Radon-Nikodym density is given by (39) and the path-integral representation (42) is apparently valid for the involved [compare, e.g., (4) again] Feynman-Kac kernel. Except for the set of measure zero, the process $X(t)$ is characterized by the standard Brownian motion $W(t)$ ensemble of sample trajectories whose "realizations" by $X(t)$ are appropriately (Cameron-Martin or Feynman-Kac) weighted.

Although for each choice of the natural boundary $\partial\Lambda$ there is a unique diffusion which respects it, we can devise a method of foliating the set of all considered diffusion processes into dynamically equivalent classes. We shall call diffusion processes dynamically equivalent if they generate the same *a priori* given field of local accelerations $b\nabla b + D\Delta b = \nabla\Omega$ in their domain of definition. It amounts to making a definite functional choice for $\nabla\Omega(x)$, $x \in R^1$, and then classifying all natural boundaries which are consistent with this choice (let us emphasize that $\frac{1}{2}b^2 + D\nabla b = \Omega$ is to hold true modulo a constant).

Following Ref. [8] we can always consider a given, unrestricted in R^1 Smoluchowski diffusion, as the reference one. Let $\Omega(x)$ be its auxiliary potential and $\nabla\Omega$ the induced field of local accelerations. What are the diffusion processes with natural boundaries which are dynamically equivalent to this reference one?

On purely technical grounds, the answer is simultaneously provided in the framework of Nelson's stochastic mechanics [4,7,8,10,14,25–29,49,44,50–53,58] and Zambrini's Euclidean quantum mechanics [7,8,50–53,58,59]. The pertinent homogeneous diffusion processes belong to the overlap of these two theoretical schemes and are uniquely specified by the nodal structure of stationary solutions of the Schrödinger-type equation: with D replacing $\hbar/2m$ in the original quantum evolution problem and the Schrödinger potential being equal to $\Omega(x)$ modulo, an additive (renormalization) constant. The ground-state process would correspond to the chosen Smoluchowski diffusion.

Example: The notorious (albeit exceptional) harmonic attraction. Let us consider the Sturm-Liouville problem on $L^2(R^1)$

$$-D\Delta\psi + \frac{\omega^2 x^2}{4D}\psi = \epsilon\psi \ . \tag{46}$$

The substitutions $\alpha^4 = \omega^2/4D^2$, $\lambda = \epsilon/\omega$, and $x = \xi/\alpha$ give rise to the equivalent eigenvalue problem

$$\left[-\frac{1}{2}\Delta_\xi + \frac{\xi^2}{2}\right]\phi = -\lambda\phi \ , \qquad \phi(\xi) = \psi\left[\frac{\xi}{\alpha}\right] = \psi(x) \ , \tag{47}$$

with the well-known solution (normalized relative to x)

$$\lambda_n = n + \tfrac{1}{2} \leftrightarrow \epsilon_n = (n + \tfrac{1}{2})\omega \ , \quad n = 0,1,2,\dots$$
$$\psi_n(x) = \phi_n(\xi) = \left[\frac{\alpha}{2^n n! \sqrt{\pi}}\right]^{1/2} \exp\left[-\frac{\xi^2}{2}\right] H_n(\xi) \ , \tag{48}$$
$$H_0 = 1, \quad H_1 = 2\xi \ ,$$
$$H_2 = 2(2\xi^2 - 1), \quad H_3 = 4\xi(2\xi^2 - 3), \ \dots \ .$$

Except for $n = 0$ the solutions $\phi_n(\xi)$ are not positive definite and change sign at nodes. We have

$n = 0$, $\psi_0(x) > 0$, $x \in (-\infty, +\infty)$;

$n = 1$, $\psi_1(x) > 0$, $x \in (0, +\infty)$;

$\psi_1(x) < 0$, $x \in (-\infty, 0)$;

$n = 2$, $\psi_2(x) > 0$, $x \in (-\infty, -1/\sqrt{2}) \cup (1/\sqrt{2}, +\infty)$;

$\psi_2(x) < 0$, $x \in (-1/\sqrt{2}, +1/\sqrt{2})$;

$n = 3$, $\psi_3(x) > 0$, $x \in (-\sqrt{3/2}, 0) \cup (\sqrt{3/2}, \infty)$;

$\psi_3(x) < 0$, $x \in (-\infty, -\sqrt{3/2}) \cup (0, \sqrt{3/2})$;

and so on. It is convenient to continue further considerations with respect to the rescaled $\xi = \alpha x$ variables, in view of the form $-\frac{1}{2}\Delta_\xi + \xi^2/2 = H$ of the Hamiltonian predominantly used in the mathematical physics literature [12]. To proceed in this notational convention it is enough to set $x \to \xi$ and $D \to \frac{1}{2}$ in the formulas (1)–(12) and thus utilize $b = \nabla\Theta/\Theta$, $\Omega = \frac{1}{2}(b^2 + \nabla b)$, and $\nabla\Omega = b\nabla b + \frac{1}{2}\Delta b$.

Although in (1)–(12) we need Θ, Θ_* of the same sign and $\rho(x)$ to be strictly positive, we can first make a formal identification $\Theta = \Theta_* = \phi_n$, $n = 0,1,2,\dots$, and notice that

$$n = 0 \ , \quad b_0 = -\xi \to \Omega_0 = \frac{\xi^2}{2} - \frac{1}{2} \ ;$$
$$n = 1 \ , \quad b_1 = \frac{1}{\xi} - \xi \to \Omega_1 = \frac{\xi^2}{2} - \frac{3}{2} \ ;$$
$$n = 2 \ , \quad b_2 = \frac{4\xi}{2\xi^2 - 1} - \xi \to \Omega_2 = \frac{\xi^2}{2} - \frac{5}{2} \ ;$$
$$n = 3 \ , \quad b_3 = \frac{1}{\xi} + \frac{4\xi}{2\xi^2 - 3} \to \Omega_3 = \frac{\xi^2}{2} - \frac{7}{2} \ .$$

Obviously $\nabla\Omega_n = \xi$ for all n. Irrespective of the fact that each b_n, $n > 0$, shows singularities, the auxiliary potentials are well defined for all x and for different values of n they acquire an additive renormalization $-\lambda_n = -(n + \frac{1}{2})$.

The case of $n = 0$ is a canonical [12,22] example of the Feynman-Kac integration and the classic Mehler formula involves the Cameron-Martin-Girsanov density (39) as well. Indeed [12] the integral kernel $[\exp(-Ht)](y,x) = k(y,0,x,t)$ for $H = -\frac{1}{2}\Delta + (\frac{1}{2}x^2 - \frac{1}{2})$ is known to be given by the formula

$$k(y,0,x,t) = \pi^{-1/2}(1 - e^{-2t})^{-1/2} \times \exp\left[-\frac{x^2 - y^2}{2} - \frac{(e^{-t}y - x)^2}{2}\right] \ , \tag{49}$$

$$(e^{-Ht}\Theta)(x) = \int k(y,0,x,t)\Theta(y)dy \ ,$$

where the integrability property

$$\int k(y,0,x,t)\exp\left[\frac{x^2 - y^2}{2}\right]dy = 1 \tag{50}$$

is simply a statement [cf. (39)] pertaining to the transition density (4) of the homogeneous diffusion, which preserves the Gaussian distribution $\rho(x) = (\Theta\Theta_*)(x) = \alpha/\sqrt{\pi}\exp(-\xi^2)$.

The case $n = 1$ automatically induces the (ergodic according to Ref. [53]) decomposition of the diffusion process into two independent noncommunicating components, each being confined between the natural boundaries $(-\infty, 0)$ and $(0, \infty)$, respectively. The pertinent processes have the same Feynman-Kac weight in the general expression (45) for their probability measures. Notice that we deal here with processes on the half-line whose drift $b_1 = 1/\xi - \xi$ has a singularity of the Bessel type when the diffusion is to approach the point 0; see, e.g., Ref. [60] for a related discussion. It suggests that the construction of the probability measure on the half-line can be accomplished by directly starting from the Bessel process with natural boundaries at 0 and ∞. Namely, the rescaled form of the backward Bessel generator

$$L_a = \frac{1}{2}\Delta_\xi + \frac{1+2a}{2\xi}\nabla_\xi \tag{51}$$

with $x = \sqrt{2}\xi$, $a \geq 0$, corresponds to the transition density of the diffusion with inaccessible boundaries

$$p(t;\xi_0,\xi) = \text{const} \times \frac{\xi}{t} \exp\left[-\frac{\xi^2+\xi_0^2}{2t}\right] I_a\left[\frac{\xi\xi_0}{t}\right], \tag{52}$$

where $I_a(\alpha)$ is the modified Bessel function. A particular choice of $a = 1/2$, i.e., $I_{1/2}(\alpha) = \sqrt{2/\pi\alpha}\sinh\alpha$, provides us [in the notational convention (47)] with a conservative diffusion whose field of drifts is $b(\xi) = 1/\xi$. This diffusion process can be directly compared (in the sense of Girsanov; see [10,14,35,36,58,60,61]) to the unrestricted harmonic diffusion considered previously: the drift transformation from $1/\xi$ to $1/\xi - \xi$ induces a corresponding transformation of probability measures. Effectively it amounts to replacing in (45) the restricted (to the semiaxis) conditional Wiener measure by the conditional Bessel measure, which automatically respects the boundaries, and next evaluating the Radon-Nikodym derivative of the harmonic measure with respect to the Bessel measure. The corresponding Cameron-Martin-Girsanov (likelihood ratio) formula can be found in Ref. [10].

The decomposition into noncommunicating diffusions with natural boundaries is characteristic of all $n > 0$ solutions of (47). However, all of them induce the same local field of accelerations $\nabla\Omega(\xi) = \xi$.

Although the existence of the Feynman-Kac kernels (and thus of the transition densities and the diffusions themselves) is granted here, it is generally not easy to give analytic expressions for them. However, in view of (44), the numerical simulation of each diffusion problem encountered before is definitely in reach. Our discussion was basically one dimensional and restricted to stationary cases; nevertheless extensions to time-dependent (nonstationary) processes and to higher dimensions (much of the outlined structure is preserved) are available.

Remark 3. Let us stress that the original analysis of Schrödinger and Jamison to evaluate the stochastic process from the input and output statistics data (as revived by Zambrini [6,62,63]), referred to the case without nodal surface of the input and output probability distribution function. Zambrini himself gave [6] a construction of the solution of the corresponding Schrödinger problem with nodal surface, hence effectively with the natural boundary. Our aim was to present a new standpoint towards a better understanding of such a "singular" Schrödinger problem by limiting the discussion to time-independent drifts (cf., however, Ref. [10] for a discussion of the time-dependent case along the similar lines). The key point is then to introduce the Feynman-Kac potential, closely linked to the Onsager-Machlup potential (cf. Yasue's [64] attempt to fix a class of stochastic processes corresponding to the same OM potential, in case of nonsingular drifts). In connection with the singular drift problems, which were the main topic of the present paper, let us notice that in Ref. [65] the formalism based on the Cameron-Martin formula was developed for nonsingular Markov-Bernstein diffusion processes and the "interesting open problem...when Θ or Θ_* have zeros" was mentioned.

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