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SCHRÖDINGER'S INTERPOLATION PROBLEM THROUGH FEYNMAN–KAC KERNELS*,**

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We discuss the so-called Schrödinger problem of deducing the microscopic (basically stochastic) evolution that is consistent with given positive boundary probability densities for a process covering a finite fixed time interval. The sought for dynamics may preserve the probability measure or induce its evolution, and is known to be uniquely reproducible, if the Markov property is required. Feynman-Kac type kernels are the principal ingredients of the solution and determine the transition probability density of the corresponding stochastic process. The result applies to a large variety of nonequilibrium statistical physics and quantum situations.

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1. Feynman–Kac kernels and time adjoint pairs of parabolic equations in the description of random dynamics

The Schrödinger problem [1] of reconstructing the "most likely" interpolating dynamics which is compatible with the prescribed input-output statistics data (analyzed in terms of nowhere vanishing boundary probability densities) for a process with the time of duration $T > 0$, can be given a unique solution, [2]. For this purpose, it is necessary to define a suitable transition probability $m(A,B) = \int_A dx \int_B dy\, m(x,y)$, mapping among Borel sets $A \to B$ in time T, so that:

(a) the bi-variate density $m(x,y)$ has the boundary data $\rho_0(A)$, $\rho_T(B)$ as its marginals for all A and B,

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(b) $m(x, y)$ has the product form with a certain strictly positive and jointly continuous in all variables kernel as a factor, [2, 3]. If the respective kernel is associated with a strongly continuous dynamical semigroup, then the interpolating process is Markovian, [3, 4].

The major issue, always to be addressed is: to specify under what circumstances (possibly phenomenological, like in case of the boundary density data) the kernel can be selected as appropriate, in reference to a concrete physical situation. Clearly, the obvious and natural candidates with a direct physical appeal are the familiar Feynman–Kac kernels, [3–6].

In the physical literature a standard arena for the usage of Feynman–Kac kernels, and the related Feynman–Kac representation formula for solutions of parabolic partial differential equations, is either the Euclidean quantum theory [10, 11, 3, 12], or the statistical physics of nonequilibrium phenomena. For example, the Fokker–Planck equation, with its non-Hermitian Markov generator, is casually mapped into the parabolic evolution problem, whose (semigroup) generator is selfadjoint. Indirectly [4, 15, 5–7], through the Cameron–Martin formula, the Feynman–Kac kernels appear as an important tool of the so called stochastic analysis of measures and related stochastic processes. It is not accidental, since probability measures and their densities are involved in each of the considered frameworks and studying dynamics in terms of densities [16, 17] is a theory with much broader, both physical and mathematical range of applications, than indicated above.

The Schrödinger equation and the generalized heat equation, which is basic for the original [18] Kac formula derivation, are connected by analytic continuation in time. (We shall proceed in the notation appropriate to problems in space dimension one, although the main body of our arguments is space dimension independent). For $V = V(x), x \in R$, bounded from below, the generator $H = -2mD^2\triangle + V$ is essentially selfadjoint on a dense subset of L^2, and the quantum unitary dynamics $\exp(-iHt/2mD)$ is a final result of the analytic continuation procedure for the holomorphic [19] semigroup $\exp(-H\sigma/2mD), \sigma = s + it, s \geq 0, s \to 0$. Here, by equating $D = \hbar/2m$, the traditional notation is restored. Since the unit ball in L^2 is left invariant by the unitary dynamics, and the Born *statistical interpretation* postulate assigns to each normalized function $\psi(x,t) = [\exp(-iHt/2mD)\psi](x,0)$ a probability measure $\mu(A) = \int_A \rho(x,t)dx \leq 1$ with the density $\rho(x,t) = \psi(x,t)\overline{\psi}(x,t)$, we are quite naturaly facing the problem of the existence of the random dynamics (stochastic process) which is compatible with the given time evolution of $\rho(x,t)$, or preserves the measure in the stationary case.

Let us emphasize that it is *not* our goal to propose any probabilistic "derivation" [21] of quantum theory. Rather, we take seriously the Born postulate and attempt to draw consequences of this assumption. Its impact is not merely conceptual: the mathematical structure of the theory is affected by submitting the quantum unitary dynamics to the methods of stochastic analysis, appropriate for any standard probabilistic problem. Quite irrespectively of whether we deal with essentially classical or quantum phenomena, and whether they are intrinsically random or have merely a random appearence (like in case of deterministic derivations of the stochastic, Brownian or Ornstein–Uhlenbeck type evolutions, [24, 25, 17]).

It is clear that the Madelung decomposition $\psi(x,t) = [\exp(R+iS)](x,t)$ of a *nonzero* (on its domain of definition) solution of the Schrödinger equation (we maintain the notation D instead of $\hbar/2m$, and consider the conservative case $V = V(x)$):

$$i\partial_t\psi(x,t) = -D\triangle\psi(x,t) + \tfrac{1}{2mD}V(x)\psi(x,t)\,,$$
$$i\partial\overline{\psi}(x,t) = D\triangle\overline{\psi}(x,t) - \tfrac{1}{2mD}V(x)\overline{\psi}(x,t)\,, \tag{1}$$

where $\overline{\psi} = \exp(R - iS)$ is a complex conjugate of ψ, while $R(x,t)$, $S(x,t)$ are real functions and $\psi(x,0)$ is taken as the initial Cauchy data for equations (1), implies the validity of the coupled pair of nonlinear partial differential equations

$$\partial_t\rho(x,t) = -\nabla(v\rho)(x,t)\,,$$
$$Q(x,t) - V(x) = 2mD[\partial_t S + D(\nabla S)^2](x,t)\,, \tag{2}$$

where

$$\rho(x,t) = \overline{\psi}(x,t)\psi(x,t) = [\exp(2R)](x,t)\,,$$
$$v(x,t) = 2D\nabla S(x,t)\,,$$
$$Q(x,t) = 2mD^2\frac{\triangle\rho^{1/2}}{\rho^{1/2}}(x,t)\,. \tag{3}$$

If, instead of complex functions $\psi, \overline{\psi}$ we introduce real functions (we follow the notation of previous publications [3, 5, 6])

$$\theta(x,t) = [\exp(R+S)](x,t)\,,$$
$$\theta_*(x,t) = [\exp(R-S)](x,t)\,, \tag{4}$$

then equations (2) can be replaced by the (nonlinearly coupled via $Q(x,t)$) pair of time adjoint parabolic equations for $\theta(x,t), \theta_*(x,t)$:

$$\partial_t\theta_* = D\triangle\theta_* - \tfrac{1}{2mD}(2Q - V)\theta_*\,,$$
$$\partial_t\theta = -D\triangle\theta + \tfrac{1}{2mD}(2Q - V)\theta\,, \tag{5}$$

with the Cauchy data $\theta(x,0), \theta_*(x,0)$ fixed by the previous Madelung exponents $R(x,0), S(x,0)$. In turn, they imply the validity of the equations (2) with $\rho(x,t) = [\exp(2R)](x,t) = \theta(x,t)\theta_*(x,t)$.

On the other hand, let us notice that the adjoint pair of the Schrödinger equations (1) comes out [5–7] as a direct result of an analytic continuation in time of the temporally adjoint parabolic problem (call it Euclidean [12, 13]):

$$\partial_t \Theta_*(x,t) = D\triangle\Theta_*(x,t) - \frac{1}{2mD}V(x)\Theta_*(x,t)\,,$$
$$\partial_t \Theta(x,t) = -D\triangle\Theta(x,t) + \frac{1}{2mD}V(x)\Theta(x,t)\,, \tag{6}$$

with a suitable (the same as in (1)) potential function $V(x)$, defining a holomorphic semigroup $\exp(-tH/2mD), t \geq 0$, and thus a consistent system of solutions $\Theta_*(x,t), \Theta(x,t)$, which gives rise to the probability measure with the quantally factorized density $(\Theta\Theta_*)(x,t)$, on all (finite) time intervals run by the time parameter t. Its relevance for the standard nonequilibrium statistical physics processes, we have discussed elswhere, [5, 8].

An *indirect* effect of the analytic continuation is the mapping of the parabolic system (6) into rather complicated (nonlinear coupling) parabolic system (5) which is a mathematical, eventually probabilistic, equivalent of the Schrödinger equation. The seemingly strange form of (5) does not preclude the full-fledged stochastic analysis. In fact, the standard methods appropriate for the problem (6) need only a slight generalization to encompass the time-dependent potentials, and next some boundary data analysis to deal with the (*a priori* admitted by (1)) nodal surfaces of the probability distribution, see *e.g.* [11, 3–5, 27, 29]. Albeit, in case of (5) and (6), if (1) is not invoked at all, the time adjoint parabolic equation might look annoying for the reader unfamiliar with the properties of fundamental solutions of the parabolic equations (assuming their existence in the present context, *cf.* [3, 5]). Let us stress that there is no conflict with the traditional intuition about physically irreversible random transport phenomena.

In each of the considered problems (1), (5), (6), the probability density was naturally associated with the temporally adjoint pair of partial differential equations. Let us choose a concrete time interval $t \in [0,T]$ and consider the boundary data $\rho(x,0), \rho(x,T)$ of the respective probability density, which we demand to be *strictly positive* on their domain of definition. We are interested in deducing a *stochastic process* taking place in this time interval, which either induces a continuous propagation (is measure preserving in the stationary case) of a probability density between the boundary data, or is consistent with the time evolution of $\rho(x,t), t \in [0,T]$, if given *a priori* as in case of (1) and (5).

Since the global existence/uniqueness theorems [2, 23, 21] tell us that the pertinent processes might be Markovian, we fall into the well established framework, where for any two Borel sets $A, B \subset R$ on which the respective strictly positive boundary densities $\rho(x,0)$ and $\rho(x,T)$ are defined, the transition probability $m(A,B)$ from the set A to the set B in the time interval $T > 0$ has a density given in a specific factorized form:

$$m(x,y) = f(x)k(x,0,y,T)g(y)\,,$$
$$m(A,B) = \int_A dx \int_B dy\, m(x,y)\,,$$
$$\int dym(x,y) = \rho(x,0)\,, \int dxm(x,y) = \rho(y,T)\,. \tag{7}$$

Here, $f(x), g(y)$ are the *a priori* unknown functions, to come out as solutions of the integral (Schrödinger) system of equations (7), provided that in addition to the density boundary data we have in hands any strictly positive, continuous in space variables *function* $k(x,0,y,T)$. Our notation makes explicit the dependence (in general irrelevant) on the time interval endpoints. It anticipates an important restriction we shall impose, that $k(x,0,y,T)$ is a particular form of a strongly continuous dynamical semigroup kernel: it will secure the Markov property of the sought for stochastic process.

It is the major mathematical discovery [2, 3] that the Schrödinger system (7) of integral equations admits a unique solution in terms of two nonzero, locally integrable (*i.e.* integrable on compact sets) functions $f(x), g(y)$ of the same sign (positive, everything is up to a multiplicative constant).

If $k(y,0,x,T)$ is a particular, confined to the time interval endpoints, form of a concrete semigroup kernel $k(y,s,x,t), 0 \leq s \leq t < T$, let it be a fundamental solution associated with (6) (whose existence *a priori* is *not* granted), then there exists [3, 5–7, 15] a function $p(y,s,x,t)$:

$$p(y,s,x,t) = k(y,s,x,t)\frac{\theta(x,t)}{\theta(y,s)}\,, \tag{8}$$

where

$$\theta(x,t) = \int dyk(x,t,y,T)g(y)\,,$$
$$\theta_*(y,s) = \int dxk(x,0,y,s)f(x)\,, \tag{9}$$

which implements a consistent propagation of the density $\rho(x,t) = \theta(x,t)\theta_*(x,t)$ between its boundary versions, according to:

$$\rho(x,t) = \int p(y,s,x,t)\rho(y,s)dy\,, \tag{10}$$

$$0 \leq s \leq t < T\,.$$

For a given semigroup which is characterized by its generator (Hamiltonian), the kernel $k(y,s,x,t)$ and the emerging transition probability density $p(y,s,x,t)$ are unique in view of the uniqueness of solutions $f(x), g(y)$ of (7). For Markov processes, the knowledge of the transition probability density $p(y,s,x,t)$ for all intermediate times $0 \leq s < t \leq T$ suffices for the derivation of all other relevant characteristics.

In the framework of the Schrödinger problem the choice of the integral kernel $k(y,0,x,T)$ is arbitrary, except for the strict positivity and continuity demand. As long as there is no "natural" physical motivation for its concrete functional form, the problem is abstract and of no direct physical relevance. However, in the context of parabolic equations (5) and (6), this "natural" choice is automatically settled if the Feynman-Kac formula can be utilized to represent solutions. (Notice that in case of (5) the finite energy condition $\int[|\nabla\psi|^2+V(x)\rho(x,t)]dx < \infty$, $\rho = |\psi|^2$ secures the boundedness from below of the potential $2Q(x,t) - V(x)$, see *e.g.* [3, 21, 23]).

Indeed, in this case an unambigous strictly positive semigroup kernel which is a continuous function of its arguments, can be introduced for a broad class of (admissible [11]) potentials. Time dependent potentials are here included as well. Moreover, in Ref. [5] we have discussed a possible phenomenological significance of the Feynman–Kac potentials, as contrasted to the usual identification of Smoluchowski drifts with force fields affecting particles (up to a coefficient) in the standard theory of stochastic diffusion processes.

There is an enormous literature on the Kac integral kernel issue [10, 11, 27] based on the concept of the conditional Wiener measure. Let us however mention that strictly positive semigroup kernels generated by Laplacians plus suitable potentials are very special examples in a surprisingly rich encompassing family. The concept of the "free noise", normally characterized by a Gaussian probability distribution appropriate to a Wiener process, can be extended to all infinitely divisible probability distributions via, the well known to probabilists and mathematical physicists, Lévy–Khintchine formula, see for example [7]. It allows to expand the framework from continuous diffusion processes to jump or combined diffusion–jump propagation scenarios which are not necessarily Gaussian. All such (Lévy) processes are associated with the strictly positive dynamical semigroup kernels and the same pertains to a number of cases when the free generator (minus Laplacian in the "normal" situation) acquires a potential term, to form a nontrivial Hamiltonian of a physical problem.

In the existing probabilistic investigations [3, 12, 5, 6], based on the exploitation of the Schrödinger problem strategy, much stronger demand than any previous one was in use: guided by the observation that $k(y,s,x,t)$

must be a *function* to allow for all advantages of (7), it was generally assumed that the kernel actually *is* a fundamental solution of the parabolic equation. It means that the kernel is a function with continuous derivatives: first order-with respect to time, second order-with respect to space variables. Then, the transition probability density defined by (8) is a fundamental solution of the Fokker–Planck (second Kolmogorov) equation in the pair x, t of variables, and as such is at the same time a solution of the backward (first Kolmogorov) equation in the pair y, s. This feature was exploited in [3, 5, 6].

There is a number of mathematical subtleties involved in the fundamental solution notion, since in this case, the Feynman–Kac kernel must be a continuously differentiable function, and a solution of the parabolic equation itself. In fact, for suitable (not too bad) potentials, each fundamental solution of the parabolic equation has the Feynman–Kac representation, [27], and is both strictly positive and continuous integral kernel [10, 11]. The inverse statement is generally incorrect: Feynman–Kac kernels may have granted the existence status, even as continuous functions [11, 30], but may not be differentiable, and need not to be solutions of any conceivable partial differential equations. Even, if the Feynman–Kac path integral representation applies to explicit solutions of the parabolic equations, which are generated from the smooth initial data by the strongly continuous semigroup action of the type $[\exp(-tH/2mD)f](x) = \theta_*(x,t)$, compare *e.g.* Eq. (9).

To our knowledge, this complication in the study of Markovian representations of the Schrödinger interpolating dynamics (and the quantum Schrödinger picture dynamics in particular) for the first time has been addressed and solved in Ref. [8].

As well, the subject of the (continuous) differentiability of Feynman–Kac kernels seems to have been left aside, also in the specialized monographs [10, 11, 27]. Nevertheless, we can firmly repeat the conclusion of our previous paper [6] that to give a definite (unique) Markov solution of the Schrödinger stochastic interpolation problem, in particular for the case of the Schrödinger picture quantum dynamics (1), a suitable (compatible with (5)) Feynman–Kac semigroup with its strictly positive and continuous in all variables kernel *must* be singled out. As it appears, the kernel may not be a fundamental solution of a parabolic equation. Anyway, for each chosen kernel, the associated Markov process is defined uniquely by (7)–(8), though *not* in reverse.

2. When diffusion processes ?

The strategy of deducing a probabilistic solution of the Schrödinger boundary data problem in terms of Markov stochastic processes running in continuous time, was accomplished in Ref. [8] in a number of steps accompanied by the gradual strengthening of restrictions imposed on the Feynman–Kac potential. To deal with the commonly accepted diffusion process notion, certain additional restrictions need to be imposed to guarrantee that the mean and variance of the infinitesimal displacements of the continuous process have the standard meaning of the drift and diffusion coefficient, respectively, [32].

According to the general wisdom, diffusions arise in conjunction with the parabolic evolution equations, since then only the conditional averages are believed to make sense in the local description of the dynamics. It is not accidental that forward parabolic equations (6) are commonly called the generalized diffusion equations. Also, the fact that the Feynman–Kac formula involves the integration over sample paths of the Wiener process, seems to suggest some diffusive features of the Schrödinger interpolation, even if we are unable to establish this fact in a canonical manner.

Clearly, the conditions valid for any $\varepsilon > 0$:

(a) there holds $\lim_{t\downarrow s} \frac{1}{t-s} \int_{|y-x|>\varepsilon} p(y,s,x,t)dx = 0$,

(b) there exists a drift function

$$b(x,s) = \lim_{t\downarrow s} \frac{1}{t-s} \int_{|y-s|\le\varepsilon} (y-x)p(x,s,y,t)dy,$$

(c) there exists a diffusion function

$$a(x,s) = \lim_{t\downarrow s} \frac{1}{t-s} \int_{|y-x|\le\varepsilon} (y-x)^2 p(x,s,y,t)dy,$$

are conventionally interpreted to define a diffusion process, [32].

If we exploit the propagation formula for $\rho(x,t)$, (10) and ask for the circumstances under which $\rho(x,t)$ is a solution of a suitable (Fokker–Planck) parabolic differential equation, it appears (see *e.g.* chap. 4.4 in Ref. [32]), that the above conditions (a), (b), (c) appear to be sufficient but *not* necessary to achieve this goal. Obviously, they can be satisfied if $p(y,s,x,t)$ is a fundamental solution.

Usually, one accepts that sample paths of the Wiener process are continuous with probability one and makes a *kinematical* assumption, [21, 20], (proposal, according to [23]) by considering only these processes with continuous trajectories which can be derived by suitable modifications of the Wiener noise, and thus are regarded as being of diffusive type from the beginning. It is at this point, where the modern theory of stochastic differential equations and related probability measures intervenes, [27, 4, 5, 23].

Then, an absolute continuity of measures relative to the Wiener one, allows for a continuous (and eventually diffusion process) realization of the Schrödinger interpolation problem. It arises in terms of weak (since an initial probability density $\rho_0(x)$ is attributed to the random variable $X(t)$) solutions $X(t) = \int_0^t b(X(s), s)ds + \sqrt{2D}W(t)$ of respective stochastic differential equations. Here, $W(t)$ stands for the standard Wiener noise, and $b(x, s)$ is a forward drift of the diffusion process. Rules of the stochastic Itô calculus allow to deduce the partial differential (Fokker–Planck or second Kolmogorov) equation governing the dynamics of the probability density (and of the transition density in particular) associated with the process.

Since, in the present framework, the Feynman–Kac semigroup kernel and the related parabolic equations (5), (6) are the principal building blocks for all the derivations, it seems instructive to indicate the standard procedures, [32, 3], linking parabolic equations with diffusion processes. All of them are based on the exploitation of fundamental solutions.

We take for granted the Feynman–Kac representation of the continuous and strictly positive kernel associated with the forward parabolic equation. Let us assume that we have given a bounded solution $u(x,t) = \int k(y, 0, x, t)u(y, 0)dz$ of (5) or (6). Let us consider $u(x,t)$ and $u(x, t+\triangle t)$, $0 \leq \triangle t \ll 1$. Since $u(x,t)$ is a solution, we have granted the existence of the time derivative and the validity of Taylor series with respect to $\triangle s$, at least to the second expansion order. The same (at least to third expansion order) applies to the Taylor expansion of $u(y,t) = u(x + (y - x), t)$ about x. Consequently:

$$u(x, t + \triangle t) = \int k(y, t, x, t + \triangle t)u(y, s)dy \simeq \int k(y, t, x, t + \triangle t)$$
$$\times \left[u(x,t) + (y - x)\nabla_x u(x,t) + \tfrac{1}{2!}(y - x)^2 \triangle_x u(x,t) + \ldots\right]dy \,. \tag{11}$$

On the other hand, we have

$$u(x, t + \triangle t) \simeq u(x,t) + \partial_t u(x,t)\triangle t \,, \tag{12}$$

and an obvious expansion, in terms of moments of the kernel $k(y, s, x, t)$ does emerge:

$$\partial_t u(x,t)\triangle t \simeq u(x, t + \triangle t) - u(x,t) \simeq -u(x,t)[1 - \int k(y, t, x, t + \triangle t)dy]$$
$$+ [\nabla_x u(x,t)] \int (y - x)k(y, s, x, t + \triangle t)dy$$
$$+ [\tfrac{1}{2!}\triangle_x u(x,t)] \int (y - x)^2 k(y, t, x, t + \triangle t)dy + \ldots \,. \tag{13}$$

Clearly, to reconcile this expansion with the forward parabolic equation obeyed by $u(x,t)$, *i.e.* $\partial_t u = -cu + \triangle u$, one needs to verify whether the correct limiting properties are respected by the Feynman–Kac kernel. In case they would hold true, the arguments of Ref. [3] would convince us that we are dealing with the diffusion process.

Presently, [8], the rigorous demonstration is available in case, when the kernel is *not* a fundamental solution of the parabolic equation.

3. From positive to nonnegative solutions of parabolic equations

Following Refs. [8, 9], let us focus our attention on stochastic Markov processes of diffusion-type (see Ref. [7] for a jump process alternative), which are associated with the general temporally adjoint pair of parabolic partial differential equations:

$$\begin{aligned} \partial_t u(x,t) &= \triangle u(x,t) - c(x,t)u(x,t)\,, \\ \partial_t v(x,t) &= -\triangle v(x,t) + c(x,t)v(x,t)\,. \end{aligned} \tag{14}$$

Here, $c(x,t)$ is a real function (left unspecified at the moment) and the solutions $u(x,t)$, $v(x,t)$ are sought for in the time interval $[0,T]$ under the boundary conditions set at the time-interval borders:

$$\begin{aligned} \rho_0(x) &= u(x,0)v(x,0)\,, \\ \rho_T(x) &= u(x,T)v(x,T)\,, \\ \int_A \rho_0(x)dx = \rho_0(A)\,, & \qquad \int_B \rho_T(x)dx = \rho_T(B)\,. \end{aligned} \tag{15}$$

We assume that ρ is a probability measure with the density $\rho(x)$, and A, B stand for arbitrary Borel sets in the event space. In the above, suitable units were chosen to eliminate inessential in the present context (dimensional) parameters, and the process is supposed to live in/on R^1.

As emphasized in the previous publications, [5–8], the key ingredient of the formalism is to specify the function $c(x,t)$ such that $\exp[-\int_0^t H(\tau)d\tau]$ can be viewed as a strongly continuous semigroup operator with the generator $H(t) = -\triangle + c(t)$, associated with the familiar [11] Feynman–Kac kernel:

$$\begin{aligned} (f, \exp[-\int_0^t H(\tau)d\tau]g) &= \int dy \int dx \overline{f}(y)k(y,0,x,t)g(x) \\ &= \int \overline{f}(\omega(0))g(\omega(t)) \exp[-\int_0^t c(\omega(\tau),\tau)d\tau]d\mu_0(\omega)\,. \end{aligned} \tag{16}$$

The exponential operator should be understood as the time-ordered expression. Here f, g are complex functions, $\omega(t)$ denotes a sample path of the conventional Wiener process and $d\mu_0$ stands for the Wiener measure. Clearly, the kernel itself can be explicitly written in terms of the conditional Wiener measure $d\mu_{(x,t)}^{(y,s)}$ pinned at space-time points (y, s) and (x, t), $0 \leq s < t \leq T$:

$$k(y, s, x, t) = \int \exp[-\int_s^t c(\omega(\tau), \tau) d\tau] \, d\mu_{(x,t)}^{(y,s)}(\omega) . \tag{17}$$

As long as we do not impose any specific domain restrictions on the semigroup generator $H(\tau)$, the whole real line R^1 is accessible to the process. Various choices of the Dirichlet [11, 5] boundary conditions can be accounted for by the formula (3). If we replace R^1 by any open subset $\Omega \subset R^1$ with the boundary $\partial\Omega$, it amounts to confining Wiener sample paths of relevance to reside in (be interior to) Ω, which in turn needs an appropriate measure $d\mu_{(x,t)}^{(y,s)}(\omega \in \Omega)$ in (4). This is usually implemented by means of stopping times for the Wiener process, [15, 5, 4, 29].

Let $f(x)$, $g(x)$ be two real functions such that: $m_T(x, y) = f(x)k(x, 0, y, T)g(y)$ defines a bi-variate density of the probability measure, *i.e.* a transition probability of the propagation from the Borel set A to the Borel set B to be accomplished in the time interval T. In particular, we need the marginal probability densities to be defined: $\rho_0(x) = m_T(x, \Omega)$, $\rho_T(y) = m_T(\Omega, y)$ where $\Omega \subset R^1$ is a spatial area confining the process.

These formulas can be viewed as special cases of (7), so establishing an apparent link between the Schrödinger problem and the Feynman–Kac kernels, together with the related parabolic equations. Assuming that marginal probability measures and their densities are given *a priori*, and a concrete Feynman–Kac kernel (17) (with or without Dirichlet domain restrictions) is specified, we are within the premises of the Schrödinger boundary data problem.

Let $\overline{\Omega} = \Omega \cup \partial\Omega$ be a closed subset of R^1, or R^1 itself. For all Borel sets (in the σ-field generated by all open subsets of $\overline{\Omega}$) we assume to have known $\rho_0(A)$ and $\rho_T(B)$, hence the respective densities as well. If the integral kernel $k(x, 0, y, T)$ in the expression (5) is chosen to be *continuous* and *strictly positive* on $\overline{\Omega}$, then the integral equations (7) can be solved [2] with respect to the *unknown* functions $f(x)$ and $g(y)$. The solution comprises two nonzero, locally integrable functions of the same sign, which are unique up to a multiplicative constant.

If, in addition, the kernel $k(y, s, x, t)$, $0 \leq s < t \leq T$ is a *fundamental solution* of the parabolic system (14) on R^1 (*i.e.* is a function which solves the forward equation in (x,t) variables, while the backward one in (y,s)), then we have defined a solution of the system (14) by:

$$u(x,t) \equiv f(x,t) = \int f(y)k(y,0,x,t)dy\,,$$
$$v(x,t) \equiv g(x,t) = \int k(x,t,y,T)g(y)dy\,. \qquad (18)$$

Moreover, $\rho(x,t) = f(x,t)g(x,t)$ is propagated by the Markovian transition probability density:

$$p(y,s,x,t) = k(y,s,x,t)\frac{g(x,t)}{g(y,s)}\,,$$
$$\rho(x,t) = \int \rho(y,s)p(y,s,x,t)dy\,,$$
$$0 \leq s < t \leq T$$
$$\partial_t \rho = \triangle\rho - \nabla(b\rho)\,,$$
$$b = b(x,t) = 2\frac{\nabla g(x,t)}{g(x,t)}\,, \qquad (19)$$

the result, which covers all traditional Smoluchowski diffusions [5, 14]. In that case, $c(x,t)$ is regarded as time-independent, and the corresponding stochastic process is homogeneous in time. The Dirichlet boundary data can be implemented as well, thus leading to the Smoluchowski diffusion processes with natural boundaries, [5]. Then, $k(y,s,x,t)$ stands for an appropriate Green function of the parabolic boundary-data problem, with the property to vanish at the boundaries $\partial\Omega$ of Ω.

Let us mention that for time-independent potentials, $c(x,t) = c(x)$ for all $t \in [0,T]$, a number of generalizations is available [15, 5, 4, 22, 29, 14, 37] to encompass the nodal sets of $\rho(x)$ and hence of the associated functions $f(x), g(x)$. The drift $b(x) = \nabla ln\rho(x) = \frac{\nabla\rho(x)}{\rho(x)}$ singularities do not prohibit the existence of a well defined Markov diffusion process (9), for which nodes are unattainable. In the considered framework they are allowed only at the boundaries of the connected spatial area Ω confinig the process.

The problem of relaxing the strict positivity (and/or continuity) demand for Feynman–Kac kernels is nontrivial [35, 36, 2] with respect to the eventual construction of the *unique* Markov process (9). To elucidate the nature of difficulties underlying this issue, we shall consider quantally motivated examples of the parabolic dynamics (14).

4. Nonlinear parabolic dynamics with unattainable boundaries

Let us choose the potential function $c(x,t)$ as follows:

$$c(x,t) = \frac{x^2}{2(1+t^2)^2} - \frac{1}{1+t^2} \tag{20}$$

for $x \in R^1, t \in [0,T]$. In view of its local Hölder continuity (*cf.* Ref.[8]) with exponent one, and its quadratic boundedness, the fundamental solution of the parabolic system is known to exist [27, 38–40]. It is constructed via the parametrix method. Among an infinity of regular solutions of (14) with the potential (20), we can in particular identify [8] solutions of the Schrödinger boundary data problem for the familiar (quantal) evolution:

$$\begin{aligned} \rho_0(x) &= (2\pi)^{-1/2} \exp\left[-\frac{x^2}{2}\right] \longrightarrow \rho(x,t) \\ &= [2\pi(1+t^2)]^{-1/2} \exp\left[-\frac{x^2}{2(1+t^2)}\right]. \end{aligned} \tag{21}$$

They read

$$\begin{aligned} u(x,t) \equiv f(x,t) &= [2\pi(1+t^2)]^{-1/4} \exp\left(-\frac{x^2}{4}\frac{1+t}{1+t^2} + \frac{1}{2}\arctan\, t\right), \\ v(x,t) \equiv g(x,t) &= [2\pi(1+t^2)]^{-1/4} \exp\left(-\frac{x^2}{4}\frac{1-t}{1+t^2} - \frac{1}{2}\arctan\, t\right), \end{aligned} \tag{22}$$

and, while solving the nonlinear parabolic system (14) (with $c = \frac{\triangle \rho^{1/2}}{\rho^{1/2}}$), in addition they imply the validity of the Fokker–Planck equation:

$$\begin{aligned} \rho(x,t) &= f(x,t)g(x,t) \to \partial_t \rho = \triangle\rho - \nabla(b\rho), \\ b(x,t) &= 2\frac{\nabla g(x,t)}{g(x,t)} = -\frac{1-t}{1+t^2}\, x. \end{aligned} \tag{23}$$

Notice that $p(y,s,x,t) = k(y,s,x,t)\frac{g(x,t)}{g(y,s)}$ is a fundamental solution of the first and second Kolmogorov (*e.g.* Fokker–Planck) equations in the present case.

Let us recall that a concrete parabolic system corresponding to solutions (22) looks badly nonlinear. Our procedure, of first considering the linear system (but with the potential "belonging" to another, nonlinear one), and next identifying solutions of interest by means of the Schrödinger boundary data problem, allows to bypass this inherent difficulty. In connection with the previously mentioned quantal motivation of ours, let us define $g = \exp(R+S), f = \exp(R-S)$ where $R(x,t), S(x,t)$ are real functions. We immediately realize that (5), (14) provide for a parabolic alternative to the familiar Schrödinger equation and its temporal adjoint:

$$i\partial_t \psi = -\triangle \psi \,, \\ i\partial_t \overline{\psi} = \triangle \overline{\psi} \,, \tag{24}$$

with the Madelung factorization $\psi = \exp(R+iS), \overline{\psi} = \exp(R-iS)$ involving the previously introduced real functions R and S.

Things seem to be fairly transparent when the parabolic system (5) or (6) allows for fundamental solutions. However, even in this case complications arise if nodes of the probability density are admitted. The subsequent discussion has a quantal origin, and comes from the free Schrödinger propagation with the specific choice, [9], of the initial data:

$$\psi_0(x) = (2\pi)^{-1/4}\, x\, \exp\left(-\frac{x^2}{4}\right) \longrightarrow \\ \psi(x,t) = (2\pi)^{-1/4} \frac{x}{(1+it)^{3/2}}\, \exp\left[-\frac{x^2}{4(1+it)}\right] \tag{25}$$

such that our nonstationary dynamics example displays a stable node at $x = 0$ for all times .

The parabolic system (1) in this case involves the potential function:

$$c(x,t) = \frac{\triangle \rho^{1/2}(x,t)}{\rho^{1/2}(x,t)} = \frac{x^2}{2(1+t^2)^2} - \frac{3}{1+t^2}\,, \\ \rho(x,t) = (2\pi)^{-1/2}(1+t^2)^{-3/2}\, x^2\, \exp\left[-\frac{x^2}{2(1+t^2)}\right]. \tag{26}$$

The polar (Madelung) factorization of Schrödinger wave functions implies:

$$R(x,t) = ln\, \rho^{1/2}(x,t)\,,$$

$$x > 0 \rightarrow S(x,t) = S_+(x,t) = \frac{x^2}{4}\frac{t}{1+t^2} - \frac{3}{2}\arctan\, t\,, \\ x < 0 \rightarrow S(x,t) = S_-(x,t) = \frac{x^2}{4}\frac{t}{1+t^2} - \frac{3}{2}\arctan\, t\, +\, \pi\,. \tag{27}$$

Although $S(x,t)$ is not defined at $x = 0$, we can introduce continuous functions $f = \exp(R-S)$ and $g = \exp(R+S)$ by employing the step function

$\varepsilon(x) = 0$ if $x \geq 0$ and $\varepsilon(x) = 1$ if $x < 0$. Then, the candidates for solutions of the parabolic system (5) with the potential (20) would read:

$$\begin{aligned} v(x,t) \equiv g(x,t) &= (2\pi)^{-1/4}(1+t^2)^{-3/4}|x| \\ &\times \exp\left(-\frac{x^2}{4}\frac{1-t}{1+t^2}\right)\exp\left[-\frac{3}{2}arctan\, t + \pi\varepsilon(x)\right], \\ u(x,t) \equiv f(x,t) &= (2\pi)^{-1/4}(1+t^2)^{-3/4}|x| \\ &\times \exp\left(-\frac{x^2}{4}\frac{1+t}{1+t^2}\right)\exp\left[\frac{3}{2}arctan\, t - \pi\varepsilon(x)\right]. \end{aligned} \tag{28}$$

For all $x \neq 0$ we can define the forward drift

$$b(x,t) = 2\frac{\nabla g(x,t)}{g(x,t)} = \frac{2}{x} - x\,\frac{1-t}{1+t^2}, \tag{29}$$

which displays a singularity at $x = 0$. Nonetheless, $(b\rho)(x,t)$ is a smooth function and the Fokker–Planck equation $\partial_t \rho = \triangle\rho - \nabla(b\rho)$ holds true on the whole real line R^1, for all $t \in [0,T]$. Notice that there is no current through $x = 0$, since $v(x,t) = 2\nabla S(x,t) = \frac{xt}{1+t^2}$ vanishes at this point for all times.

Our functions $f(x,t), g(x,t)$ are continuous on R^1, which however does not imply their differentiability. Indeed, they solve the parabolic system (5) with the potential (20) *not* on R^1 but on $(-\infty,0)\cup(0,+\infty)$. Hence, almost everywhere on R^1, with the exception of $x = 0$.

An apparent obstacle arises because of this subtlety: these functions are *not* even weak solutions of (1), because of:

$$\begin{aligned} \int_{-\infty}^{+\infty} \partial_t f(x,t)\phi(x)dx &+ \int_{-\infty}^{+\infty} \nabla f(x,t)\nabla\phi(x)dx \\ &+ \frac{1}{2}\int_{-\infty}^{+\infty} c(x,t)f(x,t)\phi(x)dx \neq 0 \end{aligned} \tag{30}$$

for every test function ϕ such that $\phi(0) \neq 0$, continuous and with support on a chosen compact set (*e.g.* vanishing beyond this set).

One more obstacle arises, if we notice that $c(x,t)$, (20) permits the existence of the unique, bounded and strictly positive fundamental solution for the parabolic system (14). Then, while having singled out a fundamental solution and the boundary density data $\rho_0(x), \rho_T(x)$ consistent with (20), we can address the Schrödinger boundary data problem associated with (2), (3):

$$u(x,0)\int k(x,0,y,T)v(y,T)dy = \rho_0(x)\,,$$
$$v(x,T)\int k(y,0,x,T)u(y,0)dy = \rho_T(x) \tag{31}$$

expecting that a unique solution $u(x,0), v(x,T)$ of this system of equations implies an identification $u(x,0) = f(x,0)$ and $v(x,T) = g(x,T)$.

However, it is not the case and our $f(x,t), g(x,t)$ do not come out as solutions of the Schrödinger problem, if considered on the whole real line R^1, on which the fundamental solution sets rules of the game. Indeed, let us assume that (31) does hold true if we choose $u(x,0) = f(x,0), v(x,T) = g(x,T)$, with f and g defined by (21). Since, in particular we have

$$g(x,T)\int k(y,0,x,T)f(y,0)dy = g(x,T)f(x,T) \tag{32}$$

then for $x \neq 0$ there holds:

$$f(x,T) = \int k(y,0,x,T)f(y,0)dy\,. \tag{33}$$

Both sides of the last identity represent continuous functions, hence the equality is valid point-wise (*i.e.* for every x). We know that $f(y,0)$ is continuous and bounded on R^1, and $k(y,0,x,T)$ is a fundamental solution of (1). Hence the right-hand-side of (33) represents a regular solution of the parabolic equation. Such solutions have continuous derivatives, while our left-hand-side function $f(x,T)$ certainly does not share this property. Consequently, our assumption leads to a contradiction and (33) is invalid in our case.

It means that the fundamental solution (*e.g.* the corresponding Feynman –Kac kernel) associated with (16) is inappropriate for the Schrödinger problem analysis, if the interpolating probability density is to have nodes (*i.e.* vanish at some points).

In our case, $x = 0$ is a stable node of $\rho(x,t)$, and is a time-independent repulsive obstacle for the stochastic process. An apparent way out of the situation comes by considering two non-communicating processes, which are separated by the unattainable barrier at $x = 0$, [29, 23, 5, 41]. The pertinent discussion can be found in [9].

5. The "Wiener exclusion"

The conventional definition of the Feynman–Kac kernel (in the conservative case)

$$\exp[-t(-\triangle + c)](y,x) = \int \exp[-\int_0^t c(\omega(\tau))d\tau]d\mu_{(x,t)}^{(y,0)}(\omega) \qquad (34)$$

comprises all sample paths of the Wiener process on R^1, providing merely for their nontrivial redistribution by means of the Feynman–Kac weight $\exp[-\int_0^t c(\omega(\tau))d\tau]$ assigned to each sample path $\omega(s) : \omega(0) = y, \omega(t) = x$.

Assume that $c(x)$ is bounded from below and locally (*i.e.* on compact sets) bounded from above. Then, the kernel is strictly positive and continuous [11].

For $c = 0$ we deal with the conditional Wiener measure

$$\begin{aligned}\exp(t\triangle)(y,x) &= \mu_{(x,t)}^{(y,0)}[\omega(s) \in R^1; 0 \le s \le t] \\ &= \mu[\omega(s) \in R^1; \omega(0) = y, \omega(t) = x; 0 \le s \le t]\end{aligned} \qquad (35)$$

pinned at space-time points $(y,0)$ and (x,t).

The previous discussion indicates that R_- is inaccessible for all sample paths originating from R_+. In reverse, R_+ is inaccessible for those from R_-. As well, we may confine the process to an arbitrary closed subset $\Omega \subset R^1$, or enforce it to avoid ("Wiener exclusion" of Ref. [30]) certain areas in R^1.

In this context, it is instructive to know that [11] for an arbitrary open set Ω, there holds:

$$\exp(t\triangle_\Omega)(y,x) = \mu_{(x,t)}^{(y,0)}[\omega(s) \in \Omega, 0 \le s \le t], \qquad (36)$$

which is at the same time a definition of the operator $-\triangle_\Omega$, *i.e.* the Laplacian with Dirichlet boundary conditions, and that of the associated semigroup kernel. This formula provides us with the conditional Wiener measure which is *confined* to the interior of a given open set, [42, 43, 5].

We can introduce an analogous measure, which is confined to the *exterior* of a given closed subset $S \subset R^1$. In case of not too bad sets (like an exterior of an interval in R^1 or a ball in R^n, the corresponding integral kernel in known [11] to be positive and continuous. Technically, if S is a (regular) closed set such that the Lebesgue measure of ∂S is zero, then:

$$\exp(t\triangle_{R\setminus S})(y,x) = \mu_{(x,t)}^{(y,0)}[\omega(s) \notin S; 0 \le s \le t]. \qquad (37)$$

The Feynman–Kac spatial redistribution of Brownian paths can be extended to cases (36), (37) through the general formula valid for any $f, g \in L^2(\Omega)$, where Ω is any open set of interest (hence $R\backslash S$, in particular):

$$(f, \exp(-tH_\Omega)g) = \int_\Omega \overline{f}(\omega(0))g(\omega(t))\exp\left[-\int_0^t c(\omega(\tau))d\tau\right]d\mu_0(\omega). \quad (38)$$

It gives rise to the integral kernel comprising the restricted Wiener path integration, which is defined at least almost everywhere in x, y. Then, its continuity is not automatically granted. We can also utilize a concept of the first exit time T_Ω for the sample path started inside Ω (or outside S)

$$T_\Omega(\omega) = inf[t > 0, X_t(\omega) \notin \Omega], \quad (39)$$

where X_t is the random variable of the process. Then, we can write, [4, 5]

$$\begin{aligned}\exp(-tH_\Omega)(y,x) &= \int \exp\left[-\int_0^t c(\omega(\tau))d\tau\right]d\mu_{(x,t)}^{(y,0)}[\omega; t < T_\Omega] \\ &= \int_\Omega \exp\left[-\int_0^t c(\omega(\tau))d\tau\right]d\mu_{(x,t)}^{(y,0)}(\omega). \quad (40)\end{aligned}$$

It is an integration restricted to these Brownian paths, which while originating from $y \in \Omega$ at time $t = 0$ are conditioned to reach $x \in \Omega$ at time $t > 0$ without crossing (but possibly touching) the boundary ∂S of S. The contribution from paths which would touch the boundary without crossing, for at least one instant $s \in [0, t]$ is of Wiener measure zero, [42].

In case of processes with unattainable boundaries, with probability 1, there is no sample path which could possibly reach the barrier at any instant $s < \infty$.

The above discussion made an implicit use of the integrability property

$$\int_0^t c(\omega(s))ds < \infty \quad (41)$$

for $\omega \in R^1, 0 \le s \le t.$, in which case the corresponding integral kernel (for bounded from below potentials) is strictly positive. Then, if certain areas are inaccessible to the process, it occurs excusively [14, 22–37] due to the drift singularities, which are capable of "pushing" the sample paths away from the barriers.

The previous procedure can be extended to the singular [44–52] potentials, which are allowed to diverge. Their study was in part motivated by the so called Klauder's phenomenon (and the related issue of the ground state degeneracy of quantal Hamiltonians), and had received a considerable attention in the literature.

In principle, if S is a closed set in R^1 like before, and $c(x) < \infty$ for all $x \in \Omega = R \backslash S$, while $c(x) = \infty$ for $x \in S$, then depending on how severe the singularity is, we can formulate a criterion to grant the exclusion of certain sample paths of the process and hence to limit an availability of certain spatial areas to the random motion. Namely, in case of (41) nothing specific happens, but if we have

$$\int_0^t c(\omega(\tau))d\tau = \infty \tag{42}$$

for $\omega(\tau) \in S$ for some $\tau \in [0,t]$, then the "Wiener exclusion" certainly appears: we are left with contributions from these sample paths only for which (42) does not occur. Unless the respective set is of Wiener measure zero.

The area Ω comprising the relevant sample paths is then selected as follows:

$$\Omega = \left[\omega; \int_0^t c(\omega(\tau))d\tau < \infty\right] \tag{43}$$

In particular, the criterion (43) excludes from considerations sample paths which cross S and so would establish a communication between the distinct connected components of Ω.

The singular set S can be chosen to be of Lebesgue measure zero and contain a finite set of points dividing R into a finite number of open connected components. With each open and connected subset $\Omega \subset R^1$ we can [44] associate a strictly positive Feynman–Kac kernel, which can be expected to display continuity.

Since the respective potentials diverge on S, their behaviour in a close neighbourhood of nodes is quite indicative. For, if ω_S is a Wiener process sample path which is bound to cross a node at $0 \le s \le t$, then the corresponding contribution to the path integral vanishes. Such paths are thus excluded from consideration. If their subset is sizable (of nonzero Wiener measure), then the eliminated contribution

$$\int_{\omega_S} \exp\left[-\int_0^t c(\omega_S(\tau))d\tau\right] d\mu_{(x,t)}^{(y,0)}(\omega) = 0 \tag{44}$$

is substantial in the general formula (35).

At the same time, we get involved a nontrivial domain property of the semigroup generator $H = -\triangle + c$ resulting in the so called ground state degeneracy [44–46]. Let us recall (Theorem 25.15 in Ref. [11]) that if c is bounded from below and locally bounded from above, then the ground state function of $H = -\triangle + c$ is everywhere strictly positive and thus bounded away from zero on every compact set.

6. Singular potentials, ground state degeneracy and the "Wiener exclusion"

Our further discussion will concentrate mainly on singular perturbations of the harmonic potential. Therefore, some basic features of the respective parabolic problem are worth invoking. The eigenvalue problem (the temporally adjoint parabolic system now trivializes):

$$-\triangle g + (x^2 - E)g = 0 = \triangle f - (x^2 - E)f \tag{45}$$

has well known solutions labeled by $E_n = 2n + 1$ with $n = 0, 1, 2, \ldots$. In particular, $g_0(x) = f_0(x) = \frac{1}{\pi^{1/4}} \exp(-\frac{x^2}{2})$ is the unique nondegenerate ground state solution. The corresponding Feynman–Kac kernel reads

$$\begin{aligned}
\exp(-tH)(y,x) =& k(y,0,x,t) = k_t(y,x) \\
=& (\pi)^{-1/2}(1 - \exp(-t))^{-1/2} \\
& \times \exp\left[-\frac{x^2 - y^2}{2} - \frac{(y\exp(-t) - x)^2}{2}\right] \\
\partial_t k =& - \triangle_x k + (x^2 - 1)k\,,
\end{aligned} \tag{46}$$

and the invariant probability density $\rho(x) = f(x)g(x) = (\pi)^{-1/2}\exp(-x^2)$ is preserved in the course of the time-homogeneous diffusion process with the transition probability density

$$p(y,s,x,t) = k_{t-s}(y,x)\frac{g(x)}{g(y)} \tag{47}$$

We have $p(y,s,x,t) = p(y,0,x,t-s)$.

Notice the necessity of the eigenvalue correction (renormalization) of the potential, both in (34) and (38), which is indispensable to reconcile the functional form of the forward drift $b(x) = 2\nabla \ln g(x) = -2x$ with the general expression for the corresponding (to the diffusion process) parabolic system potential

$$c = c(x,t) = \partial_t \ln\, g + \frac{1}{2}\left(\frac{b^2}{2} + \nabla b\right), \tag{48}$$

which equals $c(x) = x^2 - 1$ in our case.

Let us pass to the singular (degenerate) problems. The canonical (in the context of Refs. [44–49]) choice of the centrifugal potential:

$$c_E(x) = x^2 + \frac{2\gamma}{x^2} - E \tag{49}$$

generates a well known spectral solution [48, 49] for $Hg = [-\triangle + c_E(x)]g$. The eigenvalues:

$$E_n = 4n + 2 + (1 + 8\gamma)^{1/2}, \tag{50}$$

with $n = 0, 1, 2, \ldots$ and $\gamma > -\frac{1}{8} \Rightarrow (1 + 8\gamma)^{1/2} > \sqrt{2}$, are associated with the eigenfunctions of the form:

$$\begin{aligned} g_n(x) &= x^{(2\gamma+1)/2} \exp\left(-\frac{x^2}{2}\right) L_n^\alpha(x^2), \\ \alpha &= (1 + 8\gamma)^{1/2}, \\ L_n^\alpha(x^2) &= \sum_{\nu=0}^{n} \frac{(n+\alpha)!}{(n-\nu)!(\alpha+\nu)!} \frac{(-x^2)^\nu}{\nu!} \longrightarrow, \\ L_0^\alpha(x^2) &= 1, \; L_1^\alpha(x^2) = -x^2 + \alpha + 1. \end{aligned} \tag{51}$$

It demonstrates an apparent double degeneracy of both the ground state and of the whole eigenspace of the generator H. The singularity at $x = 0$ does not prevent the definition of $H = -\triangle + x^2 + \frac{2\gamma}{x^2}$ since this operator is densely defined on an appropriate subspace of $L^2(R^1)$. This singularity is sufficiently severe to decouple $(-\infty, 0)$ from $(0, \infty)$ so that $L^2(-\infty, 0)$ and $L^2(0, \infty)$ are the invariant subspaces of H with the resulting overall double degeneracy.

Potentials of the form, [11, 30, 44]:

$$c(x) = x^2 + [dist(x, \partial\Omega)]^{-3}, \tag{52}$$

where $\partial\Omega$ can be identified with ∂S, and S is a closed subset in R^1 of any (zero or nonzero) Lebesgue measure, have properties generic to the Klauder's phenomenon. Because the Wiener paths are known to be Hölder continuous of any order $\frac{1}{2} - \varepsilon, \varepsilon > 0$ and of order $\frac{1}{3}$ in particular, there holds $\int_0^t c(\omega(\tau))d\tau = \infty$ if $\omega(\tau) \in S$ for some τ. Conversely, $\int_0^t c(\omega(\tau))d\tau < \infty$ if ω never hits S. This implies that the relevant contributions to:

$$(f, \exp[-t(-\triangle + c)]g) = \int \overline{f}(\omega(0))g(\omega(t)) \exp\left[-\int_0^t c(\omega(\tau))d\tau\right] d\mu_0(\omega) \tag{53}$$

come only from the subset of paths defined by

$$Q_t = \left[\omega;\ \int_0^t c(\omega(\tau))d\tau < \infty\right]. \tag{54}$$

The above argument might seem inapplicable to the centrifugal problem. However it is not so. In the discussion of the divergence of certain integrals of the Wiener process, in the context of Klauder's phenomenon, it has been proven [51] that for almost every path from $x = 1$ to $x = -1$ (crossing the singularity point $x = 0$) there holds $\int_{t-\delta}^{t+\delta} |\omega(\tau)|^{-1}d\tau = \infty$ for any $\delta > 0$.

To be more explicit: if $\tau_1 = \tau_1(\omega)$ is the first time such that the Wiener process $W(t) = W(t,\omega)$ attains the level (location on R^1) $W(\tau_1) = 1$, then the integral over any right-hand-side neighbourhood $(\tau_1, \tau_1 + \delta)$ of τ_1 diverges:

$$\int_{\tau_1}^{\tau_1+\delta} c(\omega(t) - 1)dt = \infty \tag{55}$$

if $\int_{-1}^{+1} c(x)dx = \infty$.

In case of the left-hand-neighbourhood of τ_1, we have

$$\int_{\tau_1-\delta}^{\tau_1} c(\omega(t) - 1)dt = \infty \tag{56}$$

if $\int_{-1}^{0} xc(x)dx = \infty$.

All that holds true in case of the centrifugal potential, thus proving that the only subset of sample paths, which matters in (54) is (55). Obviously, Q_t does not include neither paths crossing $x = 0$ nor those which might hit (touch) $x = 0$ at any instant. The singularity is sufficiently severe to create an unattainable repulsive boundary for all possible processes, which we can associate with the spectral solution (50), (51).

After the previous analysis one might be left with an impression that the appearence of the stable barrier at $x = 0$ persisting for all $t \in [0, T]$, is a consequence of the initial data choice $\psi_0(0) = 0$ for the involved quantum Schrödinger picture dynamics. In general it is not so. For example, $\psi_0(x) = x^2 \exp(-x^2/4)$ which vanishes at $x = 0$, does not vanish anymore for times $t > 0$ of the free evolution. On the other hand, somewhat surprisingly from the parabolic (intuition) viewpoint, the node can be dynamically developed from the nonvanishing initial data and lead to the nonvanishing terminal data.

Let us consider, [9], a complex function:

$$\psi(x,t) = (1+it)^{-1/2} \exp\left[-\frac{x^2}{4(1+it)}\right]\left[\frac{x^2}{2(1+it)^2} + \frac{it}{1+it}\right], \tag{57}$$

which solves the free Schrödinger equation with the initial data $\psi(x,0) = \frac{x^2}{2}\exp(-\frac{x^2}{4})$. It vanishes at $x = 0$ exclusively at the initial instant $t = 0$ of the evolution.

Obviously, there is nothing to prevent us from considering

$$\Psi(x,t) = \psi(x, t-\alpha) \tag{58}$$

for $\alpha > 0$. It solves the same free equation, but with nonvanishing initial data. However, the node is developed in the course of this evolution at time $t = \alpha$ and instantaneously desintegrated for times $t > \alpha$. Here, the Schrödinger boundary data problem would obviously involve two strictly positive probability densities $\rho_0(x) = |\Psi(x,0)|^2$ and $\rho_T(x) = |\Psi(x,T)|^2$, $T > \alpha$. It would suggest to utilize the theory [8], based on strictly positive Feynman–Kac kernels, to analyze the corresponding interpolating process. However, this tool is certainly inappropriate and cannot reproduce the *a priori* known dynamics, with the node arising at the intermediate time instant.

To handle the issue by means of a parabolic system, which we can always associate with a quantum Schrödinger picture dynamics, let us evaluate the potential $c(x,t)$ appropriate for (5).

In view of

$$\rho(x,t) = \text{const}\,(1+t^2)^{-5/2} \exp\left[-\frac{x^2}{2(1+t^2)}\right]\left[\frac{x^4}{4} - x^2t^2 + t^2(1+t^2)\right], \tag{59}$$

we have (while setting $w^{1/2}(x,t) = [\frac{x^2}{4} - x^2t^2 + t^2(1+t^2)]$):

$$\begin{aligned} c(x,t) &= \frac{\triangle \rho^{1/2}(x,t)}{\rho^{1/2}(x,t)} = \frac{1}{4}\left(-\frac{x}{1+t^2} + \nabla w\right)^2 + \frac{1}{2}\left(-\frac{1}{1+t^2} + \triangle ln\, w\right) \\ &= \frac{1}{4}\frac{x^2}{(1+t^2)^2} - \frac{1}{2}\frac{3x^2 - 2t^2x}{\frac{x^4}{4} - t^2x^2 + t^2(1+t^2)} - \frac{1}{2(1+t^2)} \\ &+ \frac{1}{2}\frac{3x^2 - 2t^2}{\frac{x^4}{4} - t^2x^2 + t^2(1+t^2)} - \frac{1}{4}\left(\frac{x^3 - 2t^2x}{\frac{x^4}{4} - t^2x^2 + t^2(1+t^2)}\right)^2. \end{aligned} \tag{60}$$

The expression looks desparately discouraging, but its $t \downarrow 0$ (*i.e.* the initial data) limit is quite familiar and displays a centrifugal singularity at $x = 0$:

$$c(x,t) = \frac{\triangle \rho^{1/2}(x,0)}{\rho^{1/2}(x,0)} = \frac{x^2}{4} + \frac{2}{x^2} - \frac{5}{2}. \tag{61}$$

Since the original, dimensional expression for the centrifugal eigenvalue problem is [48]:

$$\left(-\frac{1}{2}\triangle + \frac{m^2}{2}x^2 + \frac{\gamma}{x^2}\right)g = Eg$$
$$E_n = m\left[2n + 1 + \frac{1}{2}(1+8\gamma)^{1/2}\right], \tag{62}$$

with $n = 0, 1, ...$, an obvious adjustment of constants $m = 1/2, \gamma = 1$ allows to identify $E = 5/2$ as the $n = 0$ eigenvalue of the centrifugal Hamiltonian $H = -\triangle + \frac{x^2}{4} + \frac{2}{x^2}$.

A peculiarity of the considered example is that it enables us to achieve an explicit insight into an emergence of the centrifugal singularity and its subsequent destruction (decay) for times $t > \alpha$, due to the free quantum evolution.

In view of the degeneracy of the ground-state eigenfunction $\frac{x^2}{2}\exp(-\frac{x^2}{4})$ of the centrifugal Hamiltonian, we deal here with the gradually decreasing communication between R_+ and R_-, which results in the emergence of the completely separated (disjoint) sets $(-\infty, 0)$ and $(0, +\infty)$ at $t = \alpha$, followed by the gradual increase of the communiaction for times $t > \alpha$. By "communication" we understand that the set of sample paths crossing $x = 0$ forms a subset of nonzero Wiener measure.

It also involves a generalisation (*cf.* also Refs. [8, 52, 27]) to time-dependent Feynman–Kac kernels:

$$\left(f, \exp\left[-\int_s^t H(\tau)d\tau\right]g\right) = \int \overline{f}(\omega(s))g(\omega(t))\exp\left[-\int_s^t c(\omega(\tau),\tau)d\tau\right]d\mu_0(\omega),$$
$$Q_{s,t} = \left[\omega; \int_s^t c(\omega(\tau),\tau)d\tau < \infty\right], \tag{63}$$

The finiteness condition $\int_s^t c(\omega(\tau),\tau)d\tau < \infty$, surely does not hold true, [51], if $\delta > 0$ is sufficiently small, *cf.* (60), (61).

Let us mention that some interesting mathematical questions were left aside in the present discussion. For example, even in case of conventional Feynman–Kac kernels, the weakest possible criterions allowing for their continuity in spatial variables are not yet established. An issue of the continuity of the kernel in case of general singular potentials, needs an investigation as well. The phenomenological recipes justifying the concrete choice of the kernel are not unequivocally established as yet, see *e.g.* our discussion of the Smoluchowski drift versus Feynman–Kac potential issue in Ref. [5].

REFERENCES

[1] E. Schrödinger, *Ann. Inst. Henri Poincaré* **2**, 269 (1932).
[2] B. Jamison, *Z. Wahrsch. verw. Geb.* **30**, 65 (1974).
[3] J. C. Zambrini, *J. Math. Phys.* **27**, 3207 (1986).
[4] R. Carmona, in Taniguchi Symposium , PMMP, Katata 1985, ed. K. Itô, N. Ikeda, Academic Press, Boston 1987.
[5] Ph. Blanchard, P. Garbaczewski, *Phys. Rev.* **E49**, 3815 (1994).
[6] P. Garbaczewski, R. Olkiewicz, *Phys. Rev.* **A51**, 3445 (1995).
[7] P. Garbaczewski, J.R. Klauder, R. Olkiewicz, *Phys. Rev.* **E51**, 4114 (1995).
[8] P. Garbaczewski, R. Olkiewicz, Feynman–Kac Kernels in Markovian Representations of the Schrödinger Interpolating Dynamics, *J. Math. Phys.* **37**, (1996), in press.
[9] Ph. Blanchard, P. Garbaczewski, R. Olkiewicz, Nonnegative Feynman–Kac Kernels in Schrödinger's Interpolation Problem, submitted for publication.
[10] J. Glimm, A. Jaffe, *Quantum Physics: A Functional Integral Point of View*, Springer-Verlag, Berlin 1981.
[11] B. Simon, *Functional Integration and Quantum Physics*, Academic Press, New York 1979.
[12] J.C. Zambrini, *Phys. Rev.* **A35**, 3631 (1987).
[13] J.C. Zambrini, in Ref. [17] From Quantum to Probability Theory and Back.
[14] P. Garbaczewski, *Phys. Lett.* **A178**, 7 (1993).
[15] M. Nagasawa, *Prob. Theory Relat. Fields* **82**, 109 (1989).
[16] A. Lasota, M. C. Mackey, *Chaos, Fractals, and Noise: Stochastic Aspects of Dynamics*, Springer-Verlag, Berlin 1994.
[17] *Chaos — the Interplay Between Stochastic and Deterministic Behaviour*, Karpacz'95 Winter School Proc., eds. P. Garbaczewski, M. Wolf, A. Weron, LNP vol. 457, Springer-Verlag, Berlin 1995.
[18] M. Kac, *Probability and Related Topics in Physical Sciences*, Interscience Publ., London 1957.
[19] J.A. van Casteren, *Generators of Strongly Continuous Semigroups*, Pitman, Boston 1985.
[20] E. Nelson, *Dynamical Theories of Brownian Motion*, Princeton University Press, Princeton 1967.
[21] E. Nelson, *Quantum Fluctuations*, Princeton University Press, Princeton 1985.

[22] Ph. Blanchard, Ph. Combe, W. Zheng, *Mathematical and Physical Aspects of Stochastic Mechanics*, LNP vol. 281, Springer-Verlag, Berlin 1987.
[23] E. Carlen, *Commun. Math. Phys.* **94**, 293 (1984).
[24] C. Beck, *Physica* **A169**, 324 (1990).
[25] G. Trefan, P. Grigolini, B. West, *Phys. Rev.* **A45**, 1249 (1992).
[26] T. C. Wallstrom, *Phys. Rev.* **A49**, 1613 (1994).
[27] M. Freidlin, *Functional Integration and Partial Differential Equations*, Princeton University Press, Princeton 1985.
[28] P. Garbaczewski, *Phys. Lett.* **A172**, 208 (1993).
[29] Ph. Blanchard, S. Golin, *Commun. Math. Phys.* **109**, 421 (1987).
[30] B. Simon, *Bull. Amer. Math. Soc.* **7**, 447 (1982).
[31] E. B. Dynkin, *Theory of Markov Processes*, Pergamon Press, Oxford 1960.
[32] W. Horsthemke, R. Lefever, *Noise-Induced Transitions*, Springer-Verlag, Berlin 1984.
[33] P. Garbaczewski, *Phys. Lett.* **A185**, 149 (1994).
[34] S. Bernstein, *Verh. Intern. Math. Kongr.* (Zürich), 288 (1932).
[35] R. Fortet, *J. Math. Pures Appl.* **9**, 83 (1940).
[36] A. Beurling, *Ann. Math.* **72**, 189 (1960).
[37] M. Fukushima, in: *Mathematics + Physics*, ed. L.Streit, World Scientific, Singapore, 1985, vol. 1.
[38] A.M. Ilin, A.S. Kalashnikov, O.A. Oleinik, *Usp. Mat. Nauk* **27**, 65 (1962), in Russian.
[39] M. Krzyżański, A. Szybiak, *Lincei-Rend. Sc. fis. mat. e nat.* **28**, 26 (1959).
[40] P. Besala, *Ann. Polon. Math.* **29**, 403 (1975).
[41] S. Albeverio, R. Høegh-Krohn, *Z. Warsch. verw. Geb.* **40**, 1 (1977).
[42] J. Ginibre, in: *Statistical Mechanics and Field Theory*, ed. C. DeWitt, R. Stora, Gordon and Breach, New York 1971.
[43] O. Bratteli, D. W. Robinson, *Operator Algebras and Quantum Statistical Mechanics*, Springer-Verlag, Berlin 1981, vol. II.
[44] W. Faris, B. Simon, *Duke Math. Journ.* **42**, 559 (1975).
[45] J.R. Klauder, *Acta Phys. Austr. Suppl.* **11**, 341 (1973).
[46] H. Ezawa, J.R. Klauder, L.A. Shepp, *J. Math. Phys.* **16**, 783 (1975).
[47] E. M. Harrell, *Ann. Phys.* (NY) **105**, 379 (1977).
[48] G. Parisi, F. Zirilli, *J. Math. Phys.* **14**, 243 (1973).
[49] F. Calogero, *J. Math. Phys.* **10**, 2191 (1969).
[50] B. Simon, *J. Funct. Anal.* **14**, 293 (1973).
[51] L.A. Shepp, J.R. Klauder, H. Ezawa, *Ann. Inst. Fourier-Grenoble* **24**, 189 (1974).
[52] H. Ezawa, J.R. Klauder, L.A. Shepp, *Ann. Phys.* (NY) **18**, 65 (1974).