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LANGEVIN FORMULATION OF QUANTUM DYNAMICS

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ABSTRACT

We first show that nonrelativistic quantum mechanics formulated at *imaginary*- $\hbar$ can formally be viewed as the Fokker-Planck description of a frictionless brownian motion, which occurs (in general) in an absorbing medium. We next offer a new formulation of quantum mechanics, which is basically the Langevin treatment of this brownian motion. Explicitly, we derive a *noise-average representation* for the transition probability $W(X'', t'' | X', t')$, in terms of the solutions to a Langevin equation with a gaussian white-noise. Upon analytic continuation back to *real*- $\hbar$, $W(X'', t'' | X', t')$ becomes the propagator of the original Schrödinger equation. Our approach allows for a straightforward application to quantum dynamical problems of the mathematical techniques of classical stochastic processes. Moreover, computer simulations of quantum mechanical systems can be carried out by using numerical programs based on the Langevin dynamics.

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Analogies between quantum mechanics and stochastic diffusion processes have been discovered [1] since the beginning of the quantum theory, and subsequently investigated by many authors [2]. Yet, the peculiar nature of quantum fluctuations implies that it is impossible to view quantum mechanics as a classical stochastic theory [3]. Still, the exciting possibility of handling and solving quantum dynamical problems by exploiting analytical and numerical (computer assisted) techniques of classical stochastic processes makes any work on this program well worth the effort.

A natural strategy relies upon the fact that *quantum* fluctuations become *classical* statistical fluctuations once quantum dynamics is formulated either at *imaginary-time* ($s \equiv it$) or at *imaginary- $\hbar$* ($\hbar \equiv -i\lambda$).

Consider a point particle S (mass m and no spin) with configuration space $\mathbb{R}^N$ (this is the dynamical system dealt with throughout this Letter).

Suppose first that S is described by the lagrangian

$$L_*(X, \dot{X}) = \frac{1}{2} m \dot{X}_i \dot{X}_i - \Phi_*(X) \quad (1)$$

with $\Phi_*(X)$ *time-independent*. As long as the corresponding quantum hamiltonian has a finite-energy normalizable ground-state, the imaginary-time Schrödinger equation can be written as [4]

$$\frac{\partial}{\partial s} W_*(X, s) = \left[\frac{\hbar}{2m} \frac{\partial^2}{\partial X^2} + \frac{1}{2m} \frac{\partial^2 \theta}{\partial X^2} - \frac{1}{2m\hbar} \left(\frac{\partial \theta}{\partial X_i} \right)^2 \right] W_*(X, s) \quad (2)$$

where $\theta(X)$ is the solution of the Riccati equation

$$\frac{1}{2m} \left(\frac{\partial \theta}{\partial X_i} \right)^2 - \frac{\hbar}{2m} \frac{\partial^2 \theta}{\partial X^2} - \Phi_*(X) = 0 \quad (3)$$

By further introducing the new function $P(X, s) \equiv \exp[-\theta(X)/\hbar] \cdot W_*(X, s)$, Eq.(2) becomes

$$\frac{\partial}{\partial s} P(X, s) = \left[\frac{\hbar}{2m} \frac{\partial^2}{\partial X^2} - \frac{\partial}{\partial X_i} \left(-\frac{1}{m} \frac{\partial \theta}{\partial X_i} \right) \right] P(X, s) \quad (4)$$

which is a standard Fokker-Planck equation. As a result, $P(X, s)$ can be regarded as the *probability density* of a classical stochastic diffusion process in $\mathbb{R}^N$, with diffusion constant $\hbar/2m$ and

drift velocity $-(1/m)\nabla\theta(X)$. Thus – according to *this* specific picture – quantum mechanics at imaginary–time describes a frictionless brownian motion with *conserved particle number*, which satisfies the *potential conditions* [5]. As a matter of fact, the stochastic correlation functions yield the quantum mechanical Green’s functions [6] at imaginary–time and the equal–time statistical averages give (as $s \rightarrow \infty$) the imaginary–time quantum expectations in the ground–state. All this is well known [7], along with the supersymmetric structure of the partition function [8].

Most important for us, there exists an alternative connection – more *straightforward* [9] and more *general* [10] even if much less known – between quantum theory at imaginary - $\hbar$ (equivalently imaginary–time) and classical stochastic processes.

Suppose now that S is described by the more general lagrangian

$$L(X, \dot{X}, t) = \frac{1}{2}m\dot{X}_i\dot{X}_i + \Omega_i(X, t)\dot{X}_i - \Phi(X, t) \quad (5)$$

where the potentials $\Phi(X, t)$, $\Omega(X, t)$ are assumed to be even and odd, respectively, under time–reversal, thereby implying time–reversal invariance of the equations of motion. (Still more general situations will be considered elsewhere.) Correspondingly, the Schrödinger equation at imaginary $-\hbar$ ($\hbar \equiv -i\lambda$) reads

$$\begin{aligned} \frac{\partial}{\partial t}W(X, t) = & \left\{ \frac{\lambda}{2m} \frac{\partial^2}{\partial X^2} - \frac{\partial}{\partial X_i} \left(-\frac{1}{m} \Omega_i(X, t) \right) \right. \\ & \left. - \frac{1}{\lambda} \left[\frac{\lambda}{2m} \frac{\partial \Omega_i}{\partial X_i} - \frac{1}{2m} \Omega_i(X, t) \Omega_i(X, t) - \Phi(X, t) \right] \right\} W(X, t) . \end{aligned} \quad (6)$$

Setting further

$$V_i(X, t)W(X, t) \equiv -\frac{1}{m}\Omega_i(X, t)W(X, t) - \frac{\lambda}{2m} \frac{\partial W}{\partial X_i} , \quad (7a)$$

$$\mathcal{D}(X, t) \equiv \frac{1}{\lambda} \left[\frac{\lambda}{2m} \frac{\partial \Omega_i}{\partial X_i} - \frac{1}{2m} \Omega_i(X, t) \Omega_i(X, t) - \Phi(X, t) \right] \quad (7b)$$

Eq.(6) takes the form

$$\frac{\partial}{\partial t}W(X, t) = -\frac{\partial}{\partial X_i} [V_i(X, t)W(X, t)] - \mathcal{D}(X, t)W(X, t) . \quad (8)$$

We stress that we are going to work throughout at *imaginary*– $\hbar$ (real λ). Our point of view is to interpret [11] $W(X, t)$ as the *probability density* to find S in X at time t . Accordingly, the

transition probability $W(X'', t'' | X', t')$ – propagator of Eq. (6) – enjoys the generalized Wiener–Onsager–Machlup [12] path–integral representation

$$W(X'', t'' | X', t') \sim \int \mathcal{D}X \delta(X'' - X(t'')) \delta(X' - X(t')) \exp \left\{ - (1/\lambda) \int_{t'}^{t''} dt \left[\frac{1}{2} m \dot{X}_i \dot{X}_i + \Omega_i(X, t) \dot{X}_i - \Phi(X, t) \right] \right\} \quad (9)$$

where the exponential on the r.h.s. of Eq.(9) is a (nonnormalized) *probability distribution* $P[X(t)]$ on the space $C(X', t'; X'', t'')$ of all continuous paths $X(t)$ in $\mathbb{R}^N$ with fixed end–points $X(t') = X'$, $X(t'') = X''$. Now, a glance at Eqs.(7a), (8) shows that the imaginary– $\hbar$ quantum dynamics corresponding to Lagrangian (5) can formally be viewed as the Fokker–Planck description in $\mathbb{R}^N$ of a frictionless brownian motion with diffusion constant $\lambda/2m$ and drift velocity $-(1/m)\Omega(X, t)$. Moreover, this stochastic diffusion process – performed by S – occurs in a medium where particles can be *absorbed* and *emitted*, with killing rate given by $\mathcal{D}(X, t)$ in Eq.(7b). Notice that the *potential conditions* are no longer obeyed (in general).

We present a *new formulation* of quantum mechanics based on this scenario – it is formally the Langevin description of the brownian motion in question. Specifically, we offer a *noise–average representation* for the transition probability $W(X'', t'' | X', t')$, in terms of the solutions to a Langevin equation with a gaussian white–noise. Obviously, the analytic continuation of $W(X'', t'' | X', t')$ back to *real– $\hbar$* yields the propagator of the original Schrödinger equation [13].

Actually, we want to formulate quantum dynamics at imaginary– $\hbar$ as a classical stochastic diffusion process $\xi(t)$ in $\mathbb{R}^N$ *defined* by the probability density $W(X, t)$ and the transition probability $W(X'', t'' | X', t')$ ($\xi(t)$ describes the random position of S in this picture).

As a preliminary step, consider the case where the potentials obey the condition

$$\frac{\lambda}{2m} \frac{\partial \Omega_i}{\partial X_i} - \frac{1}{2m} \Omega_i(X, t) \Omega_i(X, t) - \Phi(X, t) = 0 \quad (10)$$

so that the number of particles is now *conserved*, and Eq.(6) becomes

$$\frac{\partial}{\partial t} W_0(X, t) = \left[\frac{\lambda}{2m} \frac{\partial^2}{\partial X^2} - \frac{\partial}{\partial X_i} \left(-\frac{1}{m} \Omega_i(X, t) \right) \right] W_0(X, t) \quad (11)$$

which is a standard Fokker–Planck equation. Next, it follows from the general theory of stochastic processes [5],[14] that $\xi(t)$ satisfies the Langevin equation

$$\frac{d}{dt}\xi_i(t) = -\frac{1}{m}\Omega_i(\xi(t), t) + \eta_i(t) \quad (12)$$

where $\eta(t)$ is a gaussian white noise defined as

$$\langle \eta_i(t) \rangle_\eta = 0, \quad (13a)$$

$$\langle \eta_i(t) \eta_j(t') \rangle_\eta = \frac{\lambda}{m} \delta_{ij} \delta(t - t'). \quad (13b)$$

Assuming that $\eta(t)$ is odd under $t \rightarrow -t$, Eq.(12) is manifestly time–reversal invariant, so that $\xi(t)$ indeed describes a *frictionless* brownian motion [15]. Now, the transition probability between (X', t') and (X'', t'') ($t'' \geq t'$) in the case of a single, arbitrary noise realization $\eta(t)$ is obviously

$$W_0(X'', t'' | X', t')[\eta(t)] = \delta(X'' - \xi(\eta(t''), t''); X', t') \quad (14)$$

where $\xi(\eta(t), t; X', t')$ denotes the solution of Eq.(12) with initial condition $\xi = X'$ at $t = t'$. Correspondingly, the transition probability between (X', t') and (X'', t'') is

$$W_0(X'', t'' | X', t') = \langle W_0(X'', t'' | X', t')[\eta(t)] \rangle_\eta = \langle \delta(X'' - \xi(\eta(t''), t''); X', t') \rangle_\eta \quad (15)$$

which is the way the propagator of the Fokker–Planck equation arises in the context of Langevin dynamics.

Unfortunately, condition (10) turns out to be a very strong limitation for realistic situations, and so we proceed to *relax* it (thus the potentials will be free of any constraint from now on). Manifestly, absorption and emission processes are now operative, but the stochastic dynamics of S is still described by Eq.(12). Suppose that S is in X' at time t' , and again consider first the case of dynamical behaviour in the presence of a single noise sample $\eta(t)$. Correspondingly, S will start following the path $\xi(\eta(t), t; X', t')$ given by Eq.(12). Now, elementary probabilistic considerations tell that the probability for S to survive this path – without being absorbed – during the time interval $t' \leq t \leq t''$ is

$$\exp \left\{ - \int_{t'}^{t''} dt \mathcal{D}(\xi(\eta(t), t; X', t'), t) \right\}. \quad (16)$$

Recalling Eq.(14) for the motion without absorption, the transition probability between (X', t') and (X'', t'') in the presence of the single noise realization $\eta(t)$ is then

$$W(X'', t'' | X', t') [\eta(t)] = \delta(X'' - \xi(\eta(t''), t''); X', t')) \exp \left\{ - \int_{t'}^{t''} dt \mathcal{D}(\xi(\eta(t), t; X' t'), t) \right\}. \quad (17)$$

We conclude that the corresponding transition probability is given by

$$W(X'', t'' | X', t') = \langle W(X'', t'' | X', t') [\eta(t)] \rangle_\eta = \langle \delta(X'' - \xi(\eta(t''), t''); X', t')) \exp \left\{ - (1/\lambda) \int_{t'}^{t''} dt \left[\frac{\lambda}{2m} \frac{\partial \Omega_i}{\partial X_i} - \frac{1}{2m} \Omega_i(X, t) \Omega_i(X, t) - \Phi(X, t) \right] \right\} \Big|_{X=\xi(\eta(t), t; X' t')} \rangle_\eta \quad (18)$$

which is our final result, namely the *noise-average representation of the quantum mechanical propagator at imaginary- $\hbar$* (corresponding to lagrangian (5)).

As is well known, only trajectories $X(t)$ of $C(X', t'; X'', t'')$ which are Hölder functions of class one-half [16] actually contribute to the path-integral (9). Amusingly, their probability distribution $P[X(t)]$ can be expressed as a noise average involving $W(X'', t'' | X', t') [\eta(t)]$

$$P[X(t)] = \langle \delta[X(t) - \xi(\eta(t), t; X', t')] W(X'', t'' | X', t') [\eta(t)] \rangle_\eta \quad (19)$$

as it can be shown by standard manipulations.

It should be observed that essentially the same picture as discussed above can alternatively be obtained by performing a *double* analytic continuation – instead of in $\hbar$ – in t and in the potentials

$$t \longrightarrow s \equiv it \quad (20a)$$

$$\Omega_i(X, t) \longrightarrow \tilde{\Omega}_i(X, s) \equiv i \Omega_i(X, t) \quad (20b)$$

$$\Phi(X, t) \longrightarrow \tilde{\Phi}(X, s) \equiv \Phi(X, t) \quad (20c)$$

which leads to a noise-average representation of the quantum mechanical propagator at imaginary-time quite similar to Eq.(18). Remarkably enough, in this case the stochastic interpretation of Eq.(2)

can be recovered as the particular way of fulfilling the analog of Eq.(10) in a manner consistent with the *potential conditions*. Explicitly

$$\tilde{\Omega}_i(X) = -\frac{\partial\theta}{\partial X_i} \quad (21a)$$

$$\tilde{\Phi}(X) = \frac{1}{2m} \left(\frac{\partial\theta}{\partial X_i} \right)^2 - \frac{\hbar}{2m} \frac{\partial^2\theta}{\partial X^2} \quad (21b)$$

which make the imaginary–time Schrödinger equation stemming from lagrangian (5) coincide with Eq.(4).

We have outlined a new approach to nonrelativistic quantum mechanics, motivated by the analogy with macroscopic brownian motion – see Table – and based on a stochastic differential equation in physical time. A crucial point should be stressed. Contrary to the case of Nelson’s stochastic mechanics [17], the drift velocity in the Langevin equation (12) depends *only* on the *classical potentials* –not on the quantum mechanical wave function as in stochastic mechanics [18]. This fact *implies* that explicit quantum mechanical problems can be formulated and solved by using standard methods of classical stochastic processes. Moreover, computer simulations of quantum dynamical systems can be performed by employing numerical programs based on the Langevin dynamics [14] – they play a rôle alternative to the Monte Carlo technique defined in the context of the path–integral approach at imaginary–time (or imaginary- $\hbar$) [19]. We would like to anticipate that the knowledge of the *classical solution* of a specific dynamical problem brings about a *drastic simplification* in the explicit evaluation of r.h.s. of Eq.(18) – the integral becomes trivial! This and various other aspects of the strategy presented here will be discussed elsewhere.

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TABLE

QUANTUM MECHANICS	BROWNIAN MOTION
CONVENTIONAL FORMULATION	FOKKER-PLANCK FORMULATION
Density of probability amplitude as solution of the Schrödinger equation	Probability density as solution of the Fokker-Planck equation.
PATH-INTEGRAL FORMULATION (FEYNMAN)	PATH-INTEGRAL FORMULATION (WIENER, ONSAGER, MACHLUP)
Transition amplitude (propagator) as sum over random paths.	Transition probability (propagator) as sum over random paths.
PRESENT FORMULATION	LANGEVIN FORMULATION
Transition amplitude (propagator) (analytically continued to $\hbar \equiv -i\lambda$) as average over a white-noise	Transition probability (propagator) as average over a white-noise

Correspondence between the formulations of quantum mechanics
and of macroscopic brownian motion.

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