

# Derivation of the Schrödinger equation IV: Stochastic and the Langevin Equations for Quantum Mechanics

Derivação da equação de Schrödinger IV: Estocástica e equações de Langevin para Mecânica Quântica

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This is the fourth paper of a series devoted to mathematically derive the Schrödinger equation using stochastic constructs. We then show that Quantum Mechanics has a stochastic support by following two paths: we first present a stochastic derivation already known in the literature and show that it is equivalent to the characteristic function derivation, made by us in the first paper of this series. However, this approach does not furnish the true stochastic dynamics of the quantum mechanical system, but only an averaged one. We then present a new derivation of the Schrödinger equation based on Langevin equations that present all features of a true stochastic system. These two approaches then improve our understanding of Quantum Mechanics to encompass stochastic behavior.

**Keywords:** Langevin equations, Schrödinger equation, Stochastic derivation, Teaching of Quantum Mechanics.

Este é o quarto artigo de uma série dedicada a derivar matematicamente a equação de Schrödinger usando construtos estocásticos. Nós, então, mostramos que a Mecânica Quântica tem suporte estocástico seguindo dois caminhos: primeiro apresentamos uma derivação estocástica já conhecida na literatura e mostramos que ela é equivalente à derivação de função característica, feita por nós no primeiro artigo desta série. No entanto, esta abordagem não fornece a verdadeira dinâmica estocástica do sistema da mecânica quântica, mas apenas uma média. Apresentamos então uma nova derivação da equação de Schrödinger baseada nas equações de Langevin que apresentam todas as características de um verdadeiro sistema estocástico. Essas duas abordagens aprofundam nossa compreensão da Mecânica Quântica no sentido de abranger o comportamento estocástico.

**Palavras-chave:** Equações de Langevin, Equação de Schrödinger, Derivação estocástica, Ensino de Mecânica Quântica.

## 1. Introduction

This is a paper devoted to show that Quantum Mechanics has a stochastic support, and is conceived as a means to bring to completion what we have presented in papers I [1], II [2] and III [3] of this series, which has its fourth part in this article. This problem of finding a stochastic support for Quantum Mechanics is not new. Indeed this search flourished in the early 1950's [4, 5] and has a great improvement in the next two decades [6–14], being a field of investigation up to now.

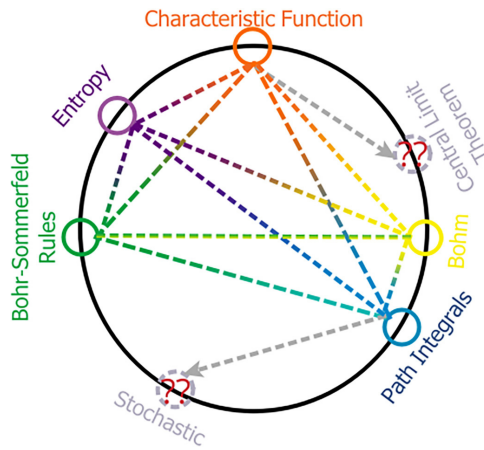
Indeed, in paper III [3], we showed that the Schrödinger equation can be derived from the axioms presented in papers I [1] and II [2], by considering sums of random variables, which we assumed as being connected with the momentum variable by making the sampling over “fibers” on phase space labelled by the configuration space coordinate  $q$ . However, as we have stressed there, at that point we have no clue whatsoever of the *equation* that will provide us with such random

variables. This, of course, calls for a dynamical equation that *must* be different from Newton's equation, since we need that the momentum be a random variable, not a deterministic one.

The usual stochastic derivations of the Schrödinger equation does not furnish this equation. In fact, as we will show, these derivations *show* us *why* the random variables do not appear in the Schrödinger equation (a mean is being taken, as we will see, that washes out these variables). We then need to search elsewhere for an equation that deals with random variables, that connects these variables to the momenta of the physical system and still recovers all the behavior of any quantum mechanical system. As we will show, these equations are the Langevin equations, modelled to give the appropriate results of usual Quantum Mechanics in the appropriate limit.

Thus, we have mathematically connected various constructs and derivations of the Schrödinger equation, as shown in Figure 1, but it still remains to show, in the sense aforementioned that the theory can also be obtained by a set of equations related to random variables, that is, that it has a stochastic support.

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**Figure 1:** The present status of our derivations and their, mathematically proven, interconnections.

To accomplish that, the paper is organized as follows: in the second section, we present one of the stochastic derivations already known in the literature, and show that this derivation has an immediate formal connection with the approach based on the characteristic function, developed in paper I of this series [1]. Then, after recognizing that the previous derivation cannot furnish a true random behavior for the physical systems, given that averages were performed, we show, in section three that it is possible to introduce a Langevin equation that gives the correct quantum mechanical description of the system and also makes it explicit the momentum random variables which can then be summed up to construct the probability density function over phase space that is the one obtained in paper II [2] of this series. This equation is quite easy to computationally simulate and we present, in section four and without entering into too much details, the results of these simulations made for some concrete quantum mechanical systems. The fifth section is devoted to our final considerations.

## 2. Stochastic Average Derivation

One can find many stochastic derivations of the Schrödinger equation in the literature [15, 16]. However, in this section we will use the stochastic derivation of de La Peña [16–18], which makes it explicit the stochastic variables and their properties. We will adapt de La Peña’s derivation to one dimension as a means to simplify it, making the didactic transposition of the approach, and because in this way it is by far a more direct derivation, and the comparison to what we have done in paper I [1] is immediate.

Thus, let us begin assuming that the velocity  $c$  of the particle is the sum of a systematic or current velocity  $v$  and a stochastic component  $u$

$$c = u + v, \tag{1}$$

and let us introduce the time inversion operator  $\hat{T}$ . We now *impose* (a first axiom) that the velocities transform under  $\hat{T}$  as

$$\hat{T}v = -v; \quad \hat{T}u = u. \tag{2}$$

Obviously, it is the random character of the stochastic velocity that makes it be invariant under time inversion. On the other hand, the first equality imposes itself since we want our formalism to imply Newtonian mechanics in the limit in which stochastic velocities are absent and, in this case, the velocity must transform as a vector under time inversion. We thus have

$$\hat{T}c = c' = -v + u, \tag{3}$$

and thus

$$v = \frac{1}{2}(c - c'); \quad u = \frac{1}{2}(c + c'). \tag{4}$$

We now need an operator that correlates the position and velocities (like  $d/dt$  in usual Newtonian mechanics). We thus *assume* that there exists a distribution of the changes in the space coordinate

$$\delta q = q(t + \delta t) - q(t), \tag{5}$$

occurring in a small time interval  $\delta t$ . Suppose now that  $f(q; t)$  is any smooth function of  $q$  and  $t$ ; we can write

$$\begin{aligned} & \frac{f(q(t + \delta t), t + \delta t) - f(q(t), t)}{\delta t} \\ & \approx \left[ \frac{\partial}{\partial t} + \frac{1}{\delta t} \delta q \frac{\partial}{\partial q} + \frac{1}{2\delta t} \delta q^2 \frac{\partial^2}{\partial q^2} + \dots \right] f(q(t), t). \end{aligned} \tag{6}$$

Taking the average of the above expression (average values with respect to the  $\delta q$  distributions) we find

$$\begin{aligned} \hat{D}f(q; t) &= \lim_{\delta t \rightarrow 0} \frac{\langle f(q(t + \delta t), t + \delta t) - f(q(t), t) \rangle}{\delta t} \\ &= \left[ \frac{\partial}{\partial t} + c \frac{\partial}{\partial q} + D \frac{\partial^2}{\partial q^2} + \dots \right] f(q; t), \end{aligned} \tag{7}$$

where  $c, 2D, \dots$  stand for the limits of the first-, second-, ... order moments of the distribution divided by  $\delta t$ , and we are identifying  $c$  with the components of the previously introduced velocity  $c$  – note that all the dependence of the equation on  $\delta q$  is now inserted in the coefficients  $c, 2D \dots$

Note that  $\hat{D} \rightarrow \partial/\partial t + c\partial/\partial q = d/dt$  in the limit when  $D \rightarrow 0$ . This operator  $\hat{D}$  gives under time inversion the result

$$\begin{aligned} \hat{D}'f(q; t) &= \hat{T}\hat{D}f(q; t) \\ &= -\frac{\partial f(q; t)}{\partial t} + c' \frac{\partial f(q; t)}{\partial q} + D' \frac{\partial^2 f(q; t)}{\partial q^2}, \end{aligned} \tag{8}$$

and we call  $\hat{D}$  the mean forward derivative operator, while we call  $\hat{D}'$  the mean backward derivative operator, since in the limit  $u \rightarrow 0$ , this operator goes into  $-d/dt$ . We end up with

$$\begin{aligned} \hat{D} &= \frac{\partial}{\partial t} + c \frac{\partial}{\partial q} + D \frac{\partial^2}{\partial q^2} + \dots \\ \hat{D}' &= -\frac{\partial}{\partial t} + c' \frac{\partial}{\partial q} + D' \frac{\partial^2}{\partial q^2} + \dots \end{aligned} \tag{9}$$

and we note that we readily have

$$\hat{D}q = c; \quad \hat{D}'q = c', \tag{10}$$

which implies that

$$\begin{aligned} v &= \frac{1}{2} (\hat{D} - \hat{D}')q = \hat{D}_c q \\ u &= \frac{1}{2} (\hat{D} + \hat{D}')q = \hat{D}_s q \end{aligned}, \tag{11}$$

where  $\hat{D}_c$  is the current derivative operator and  $\hat{D}_s$  is the stochastic derivative operator. Using (9) these new operators may be written as

$$\begin{aligned} \hat{D}_c &= \frac{\partial}{\partial t} + v \frac{\partial}{\partial q} + D_- \frac{\partial^2}{\partial q^2} + \dots \\ \hat{D}_s &= u \frac{\partial}{\partial q} + D_+ \frac{\partial^2}{\partial q^2} + \dots \end{aligned}, \tag{12}$$

where  $D_+ = (D + D')/2$  and  $D_- = (D - D')/2$ . We note that  $\hat{D}_s q = 0$  in the Newtonian limit, since Newtonian physics has no stochastic variable.

We now need to introduce a force to build a dynamic theory. We follow Newton's prescription and *assume* (another axiom) that the acceleration is given by

$$a = \hat{D}c, \tag{13}$$

and is calculated as the forward derivative of the general velocity. This means that we have

$$a = \hat{D}_c v + \hat{D}_s u + \hat{D}_c u + \hat{D}_s v \tag{14}$$

that reduces in the Newtonian limit to the known result  $a = \hat{D}_c v = dv/dt$ , which is the usual result for the total acceleration acting on the particle.

Let us consider now only  $\hat{T}$ -invariant forces (those not depending upon velocities). Since we want to identify the acceleration  $a$  with the total force acting upon our particle, we must have  $a$  as a  $\hat{T}$ -invariant quantity. However, we have that

$$\hat{D}'_c = \hat{T} \hat{D}_c = -\hat{D}_c; \quad \hat{D}'_s = \hat{T} \hat{D}_s = \hat{D}_s, \tag{15}$$

and thus

$$\hat{T}a = \hat{D}_c v + \hat{D}_s u - \hat{D}_c u - \hat{D}_s v, \tag{16}$$

which means that

$$\hat{D}_c v + \hat{D}_s u = a; \quad \hat{D}_c u + \hat{D}_s v = 0. \tag{17}$$

Now, we may identify the total force  $f$  with our acceleration  $a$  as  $f = ma$ . If we put

$$a = a_c + a_s, \tag{18}$$

where

$$\begin{aligned} a_c &= D_c v = D_c^2 q = \hat{T} a_c = a'_c \\ a_s &= D_s u = D_s^2 q = \hat{T} a_s = a'_s \end{aligned}, \tag{19}$$

showing that the current changes of  $u$  are always compensated by the changes impressed by the stochastic motion on  $v$ , because of the second equation in (17).

Our last postulate for this approach is given by the association of the *external* force with a combination of current and stochastic accelerations in the form

$$f_0 = m(\lambda_1 a_c - \lambda a_s), \tag{20}$$

and since the *total* force is given by  $f = m(a_c + a_s)$ , we may write  $f$  as a linear combination of the external force and  $a_s$ . From space time translation symmetry, we conclude that  $\lambda_1$  and  $\lambda$  must be constants and, since we search for an equation that reproduces Newtonian mechanics in the limit  $a_s \rightarrow 0$ , we must have  $\lambda_1 = 1$  and, thus,

$$f_0 = m(a_c - \lambda a_s); \quad f = f_0 + m(\lambda + 1) a_s. \tag{21}$$

Equations (17) and (21) imply that our system is described by

$$\begin{aligned} f_0 &= m(\hat{D}_c v - \lambda \hat{D}_s u) \\ \hat{D}_c u + \hat{D}_s v &= 0 \end{aligned}, \tag{22}$$

and using the operators (12) we may write these equations more explicitly as

$$\begin{aligned} \frac{\partial v}{\partial t} + v \frac{\partial v}{\partial q} + D_- \frac{\partial^2 v}{\partial q^2} - \lambda u \frac{\partial u}{\partial q} - \lambda D_+ \frac{\partial^2 u}{\partial q^2} + \dots &= f_0/m \\ \frac{\partial u}{\partial t} + v \frac{\partial u}{\partial q} + D_- \frac{\partial^2 u}{\partial q^2} + u \frac{\partial v}{\partial q} + D_+ \frac{\partial^2 v}{\partial q^2} + \dots &= 0 \end{aligned}, \tag{23}$$

which are our primary equations.

Equations (23) can be written as

$$\begin{aligned} \frac{\partial v}{\partial t} + \frac{\partial}{\partial q} \left[ \frac{v^2}{2} + D_- \frac{\partial v}{\partial q} - \lambda \frac{u^2}{2} - \lambda D_+ \frac{\partial u}{\partial q} \right] \\ + \dots = -\frac{1}{m} \frac{\partial V}{\partial q}, \tag{24} \\ \frac{\partial u}{\partial t} + \frac{\partial}{\partial q} \left[ uv + D_- \frac{\partial u}{\partial q} + D_+ \frac{\partial v}{\partial q} \right] + \dots = 0 \end{aligned}$$

which is the system of equations that we will show as equivalent, under some assumptions, to the Schrödinger equation. In fact, when imposing certain conditions upon the previous equation to recover the Schrödinger equation we will get, precisely, the connection between

the present approach and the characteristic function derivation of the Schrödinger equation.

Indeed, looking at the equations that lead to the Schrödinger equation in paper I [1], if we write

$$v = \frac{1}{m} \frac{\partial S(q;t)}{\partial q}; \quad u = 2D_0 \frac{\partial \ln R(q;t)}{\partial q}, \quad (25)$$

where  $R(q;t)$  and  $S(q;t)$  are real dimensionless functions of  $q$  and  $t$ , and put  $D=0$ ,  $D_+ = D = \hbar/2m$ ,  $\lambda = 1$ , to get

$$\begin{aligned} \frac{\partial S(q;t)}{\partial t} + V(q) + \frac{1}{2m} \left( \frac{\partial S}{\partial q} \right)^2 - \frac{\hbar^2}{2mR} \frac{\partial^2 R(q;t)}{\partial q^2} &= 0 \\ \frac{\partial R(q;t)^2}{\partial t} + \frac{\partial}{\partial q} \left[ \frac{R(q;t)^2}{m} \frac{\partial S}{\partial q} \right] &= 0 \end{aligned}, \quad (26)$$

As we have already noted in paper I [1], the two equations in (26) are equivalent to the Schrödinger equation if we replace  $\psi(q;t)$  by

$$\psi(q;t) = R(q;t) \exp \left( \frac{iS(q;t)}{\hbar} \right), \quad (27)$$

and separate into real and imaginary parts.

One of the most important expressions of this section is (25), which we rewrite here as

$$\begin{aligned} u(q;t) &= \frac{\hbar}{m} \frac{\partial \ln R(q;t)}{\partial q} \\ &= \frac{\hbar}{2m} \frac{\partial \ln \rho(q;t)}{\partial q} = \frac{\hbar}{2mk_B} \frac{\partial \mathfrak{S}(q;t)}{\partial q}, \end{aligned} \quad (28)$$

where we put, as usual,  $\rho(q;t) = R^2(q;t)$  and wrote  $\mathfrak{S}(q;t) = k_B \ln \rho(q;t)$  for the entropy. This last equation associates the stochastic velocity with the derivative of the entropy, which is precisely the content of the fluctuation-dissipation theorem (see [19], pp. 594–597).

### 2.1. Some qualifications on the derivation

The previous derivation is, at least for its one dimensional representation, quite simple and the relation between it and the developments of paper I [1] are immediate. This relation brings about some new understandings that were hidden in the characteristic function derivation of paper I.

Indeed, now we were able to write down explicitly the stochastic variables of the approach, the stochastic velocity and acceleration, and furnish their formal expression, as shown in (28).

Furthermore, this relation also makes explicit the necessary use of Boltzmann's entropy, a concept used in the entropy derivation of the Schrödinger equation, done in paper II [2].

We thus learn, with the present derivation, that we were, in all the previous derivations already presented [1–3] dealing with a stochastic approach, something that

we can say only now, that this feature of the derivation was mathematically presented.

On the other hand, our previous derivations also gives us important understandings about the stochastic derivation so far presented. For instance, we already *know*, from paper III [3] and the Central Limit Theorem, that expression (6), and all the equations that followed it, *are not* approximations.

We get those new results at the price of having a more involved derivation, that used many suppositions as a means to get to the searched result.

Moreover, equation (6) makes it clear that we are working within the realm of a stochastic system after making an average on the dynamical behavior of the system, something that becomes obvious in all derivations, in particular in the derivation in paper II [2] and also in [20, 21]. In any case, we show, once more, that Bohmian Quantum Mechanics has a statistical (now stochastic) support and cannot be considered a deterministic approach to Quantum Mechanics [22].

In fact, the average previously mentioned makes it difficult to appreciate the explicit stochastic behavior of the problem and, in fact, this stochastic behavior is hidden in the Schrödinger equation exactly because of this average. Thus, the stochastic velocity for a quantum mechanical system, according to (28), will be a *deterministic* function  $u(q,t)$ , while one would expect, for a thorough stochastic approach, to find a true random system with trajectories that are *realizations* given by the action of a truly random force.

Such an approach, which is another stochastic derivation of the Schrödinger equation, is presented in the next section.

## 3. Stochastic Langevin Derivation

In this section we will show that it is possible to find a true stochastic equation for Quantum Mechanics in the form of a Langevin equation [23]. This result, thus, complements the one obtained in previous sections, and also fulfill the necessities of paper III [3], where we derived the Schrödinger equation using the Central Limit Theorem *without knowing which equation would furnish the sums of random variables that the theorem assumes*.

Thus, let us begin with a two-dimensional system (phase-space of a system with one degree of freedom) for which our proposed Langevin equations are given by

$$\begin{cases} \frac{dp(t)}{dt} = -\gamma p(t) + \phi_1(q) + \sqrt{\Gamma_{22}(q)} \zeta(t) \\ \frac{dq(t)}{dt} = \frac{1}{m} p(t) \end{cases}, \quad (29)$$

where the second term on the right hand side of (29) gives the average behavior of the field subsystem, the third and first terms give, respectively, the fluctuation

profile of the phenomenon and the dissipation of such fluctuations, such that

$$\langle \zeta(t) \rangle = 0; \quad \langle \zeta(t) \zeta(t') \rangle = \delta(t - t'). \quad (30)$$

The first equation in (29) may be solved by the usual method: *over the fiber defined by q* we first make the discretization of the time to find

$$p_{n+1} = ap_n + \tau\phi_1(q) + \sqrt{\tau\Gamma_{22}(q)}\xi_n, \quad (31)$$

$$\zeta(t) \rightarrow \frac{1}{\sqrt{\tau}}\xi_n, \quad (32)$$

such that

$$\langle \xi_n \rangle = 0; \quad \langle \xi_n \xi_m \rangle = \delta_{n,m}. \quad (33)$$

Note that we have not iterated in the variable  $q$ ; this is because we are searching for the momentum probability distribution *for each point in the configuration space*. Thus, for each such point  $q$ ,  $p_n$  is a random variable that we can consider using the traditional statistical methods.

This is equivalent to treating the phase-space as a set of fiber bundles with width  $\delta q$ , centered in each point  $q$  of the configuration space, an approach with which we are now acquainted. The stochastic variable  $p_n$  defined above is being considered within each fiber bundle (see these arguments in greater detail in paper III [3]).

The sampling of phase-space by momentum fibers indexed by some configuration space coordinate. In the ensemble approach: we let our particles to begin at any point of the phase space and, after some definite time, given by  $n\tau$  we make our statistics over the fiber using the characteristic function given in (37).

Now, iterating (31) we find, for the first iteration

$$p_1 = ap_0 + \tau\phi_1(q) + \sqrt{\tau\Gamma_{22}(q)}\xi_0;$$

for the second iteration

$$p_2 = a^2p_0 + \tau[\phi_1(q) + a\phi_1(q)] + [\sqrt{\tau\Gamma_{22}(q)}\xi_1 + a\sqrt{\tau\Gamma_{22}(q)}\xi_0],$$

and, in general,

$$p_{n+1} = a^{n+1}p_0 + \tau \sum_{\ell=0}^n a^\ell \phi_1(q) + \sqrt{\tau} \sum_{\ell=0}^n a^\ell \sqrt{\Gamma_{22}(q)} \xi_{n-\ell}. \quad (34)$$

If we put  $p_0 = 0$  for simplicity, we get

$$p_n = \sum_{\ell=0}^{n-1} w_\ell, \quad (35)$$

where  $w_\ell$  is the random variable

$$w_\ell = \tau a^\ell \phi_1(q) + \sqrt{\tau} a^\ell \sqrt{\Gamma_{22}(q)} \xi_{n-\ell}. \quad (36)$$

Thus,  $p_n$  is the sum of independent random variables

$$Z_n(q, \delta q; t) = \left\langle \exp\left(\frac{ip_n \delta q}{\hbar}\right) \right\rangle, \quad (37)$$

where we note that, because the functions  $\Gamma_{22}$  are dependent of  $q$ , we must have the same dependence for the characteristic function  $Z_n$ . In fact, the averaging process represented in (37) is explicitly given by

$$Z_n(q, \delta q; t) = \int \exp\left(\frac{ip_n \delta q}{\hbar}\right) f(q, p_n; t) dp_n; \quad (38)$$

thus, since we write (1) as (38) with  $\delta q = 0$ ,

$$\langle 1 \rangle = \rho(q), \quad (39)$$

and we are supposing that all the variables  $p_k, q$  have the same underlying joint probability distribution function (see the derivation of the Central Limit Theorem in paper III [3]). Now, (37) may be written as

$$Z_n(q, \delta q; t) = \int \exp\left(\frac{i\delta q}{\hbar} \sum_{\ell=0}^{n-1} w_\ell\right) \prod_{\ell=0}^{n-1} f(q, w_\ell; t) dw_\ell, \quad (40)$$

which results into

$$Z_n(q, \delta q; t) = \rho(q) \prod_{\ell=0}^{n-1} \left\langle \exp\left(\frac{iw_\ell \delta q}{\hbar}\right) \right\rangle_{w_\ell}, \quad (41)$$

since the  $w_\ell$ 's are all independent random variables – note that the averages are now taken with respect to  $w_\ell$  and the characteristic function  $\left\langle \exp\left(\frac{iw_\ell \delta q}{\hbar}\right) \right\rangle_{w_\ell}$  is such that  $\langle 1 \rangle_{w_\ell} = 1$ . We also note that (remembering that our averages are now related to  $w_\ell$  alone)

$$\langle w_\ell \rangle = \tau a^\ell \phi_1(q) + a^\ell \sqrt{\tau\Gamma_{22}(q)} \langle \xi_\ell \rangle. \quad (42)$$

Using (33), we find

$$\langle w_\ell \rangle = \tau a^\ell \phi_1(q). \quad (43)$$

We also have

$$w_\ell^2 = \tau^2 a^{2\ell} \phi_1^2(q) + 2a^{2\ell} \tau^{3/2} \sqrt{\Gamma_{22}(q)} \xi_\ell + \tau a^{2\ell} \Gamma_{22}(q) \xi_\ell^2, \quad (44)$$

and, thus,

$$\langle w_\ell^2 \rangle = a^{2\ell} \tau^2 \phi_1^2(q) + \tau a^{2\ell} \Gamma_{22}(q), \quad (45)$$

where we used again the results in (33). We may also calculate

$$w_\ell^3 = \tau^3 a^{3\ell} \phi_1^3(q) + 3a^{3\ell} \tau^{5/2} \phi_1^2(q) \sqrt{\Gamma_{22}(q)} \xi_\ell + 3\tau^2 a^{3\ell} \phi_1(q) \Gamma_{22}(q) \xi_\ell^2 + \tau^{3/2} a^{3\ell} \Gamma_{22}(q)^{3/2} \xi_\ell^3, \quad (46)$$

and higher orders moments.

The variance of the random variable  $w_\ell$  becomes

$$\langle w_\ell^2 \rangle - \langle w_\ell \rangle^2 = \tau a^{2\ell} \Gamma_{22}(q), \tag{47}$$

and, thus,

$$\begin{aligned} & \left\langle \exp \left( \frac{i w_\ell \delta q}{\hbar} \right) \right\rangle_{w_\ell} \\ &= \exp \left\{ -\tau a^{2\ell} \Gamma_{22}(q) \frac{\delta q^2}{\hbar^2} \right\} \exp \left( -\frac{i \langle w_\ell \rangle \delta q}{\hbar} \right), \end{aligned} \tag{48}$$

with  $\phi_1(q) = \phi_1^2(q)$ , and we get

$$\begin{aligned} Z_n(q, \delta q; \tau) &= \rho(q) \exp \left( -\frac{b_n(q; \tau) \delta q^2}{2\hbar^2} \right) \\ &\times \exp \left( -\frac{i \bar{p}_n(q; \tau) \delta q}{\hbar} \right), \end{aligned} \tag{49}$$

where

$$b_n(q; \tau) = \tau \Gamma_{22}(q) \sum_{\ell=0}^{n-1} a^{2\ell}, \tag{50}$$

and

$$\bar{p}_n(q; \tau) = \tau \phi_1(q) \sum_{\ell=0}^{n-1} a^\ell, \tag{51}$$

where  $\bar{p}_n$  is called the average momentum; note that this nomenclature is appropriate, since  $\phi_1(q)$  is a force depending upon only the random variable  $q$  and  $\tau$  is a time, and thus  $\tau \phi_1(q)$  has the dimension of an average momentum (an impulse), for it could be explicitly written as

$$\begin{aligned} \bar{p}_n(q; \tau) \rho(q) &= \sum_{\ell=0}^{n-1} \int \tau a^\ell \phi_1(q) f(q, p_n; t) dp_n \\ &= \tau \phi_1(q) \rho(q) \sum_{\ell=0}^{n-1} a^\ell, \end{aligned} \tag{52}$$

and is usually called (in non-equilibrium kinetic theory) the macroscopic average momentum [39] (see also paper II [2]).

Expression (49) automatically implies, by inversion of the Fourier transform, that

$$f(q, p_n; \tau) = \frac{\rho(q)}{\sqrt{2\pi b_n(q; \tau)}} \exp \left\{ -\frac{[p_n - \bar{p}_n(q; \tau)]^2}{2b_n(q; \tau)} \right\}, \tag{53}$$

where we have already normalized the density  $f(q, p; t)$ . Now we may take the limit  $\tau \rightarrow 0, n \rightarrow \infty$ , such that  $n\tau \rightarrow t$ , to find

$$f(q, p; t) = \frac{\rho(q)}{\sqrt{2\pi b(q; t)}} \exp \left\{ -\frac{[p - \bar{p}(q; t)]^2}{2b(q; t)} \right\}, \tag{54}$$

where

$$\begin{aligned} b(q; t) &= \lim_{\tau \rightarrow 0} \tau \Gamma_{22}(q) \sum_{\ell=0}^{n-1} a^{2\ell} \\ \bar{p}(q; t) &= \phi_1(q) \lim_{\tau \rightarrow 0} \tau \sum_{\ell=0}^{n-1} a^\ell; \end{aligned} \tag{55}$$

Note, however, that, since (using  $\tau = t/n$ )

$$\sum_{\ell=0}^{n-1} a^{2\ell} = \frac{1 - [(1 - \gamma t/n)^n]^2}{1 - (1 - \gamma\tau)^2} = \frac{1 - [(1 - \gamma t/n)^n]^2}{2\gamma\tau - \gamma\tau^2}, \tag{56}$$

we get

$$\lim_{\tau \rightarrow 0, n \rightarrow \infty} \tau \Gamma_{22}(q) \sum_{\ell=0}^{n-1} a^{2\ell} = \Gamma_{22}(q) \left( \frac{1 - e^{-2\gamma t}}{2\gamma} \right). \tag{57}$$

Thus, we may write

$$\begin{aligned} b(q; t) &= \Gamma_{22}(q) \left[ \frac{1 - e^{-2\gamma t}}{2\gamma} \right], \\ \bar{p}(q; t) &= \phi_1(q) \left( \frac{1 - e^{-\gamma t}}{\gamma} \right), \end{aligned} \tag{58}$$

and, for large enough times ( $t \rightarrow \infty$ ),

$$b(q) = \frac{\Gamma_{22}(q)}{2\gamma}; \quad \bar{p}(q) = \frac{\phi_1(q)}{\gamma}. \tag{59}$$

With the previous results, we find, for the asymptotic distributions,

$$f(q, p; t) = \frac{\rho(q)}{\sqrt{2\pi b(q)}} \exp \left\{ -\frac{[p - \bar{p}(q; t)]^2}{2b(q)} \right\}, \tag{60}$$

as the joint probability distribution related with the Langevin system of equations (29).

Note that, for higher order moments, we get results such as

$$\begin{aligned} \sum_{\ell=0}^n \langle w_\ell^3 \rangle &= \phi_1^3(q) \tau^3 \sum_{\ell=0}^n a^{3\ell} + 3\tau^2 \phi_1(q) \Gamma_{22}(q) \sum_{\ell=0}^n a^{3\ell} \\ &= [\phi_1^3(q) \tau^3 + 3\tau^2 \phi_1(q) \Gamma_{22}(q)] \\ &\cdot \frac{1 - \exp(-3\gamma t)}{-3\gamma\tau + 3\gamma^2\tau^2 + \gamma^3\tau^3}, \end{aligned} \tag{61}$$

which goes to zero as  $\tau \rightarrow 0$ , the same happening to orders higher than three. This means that the expression for the characteristic function  $Z(q, \delta q; t)$  using only up to second order in  $\delta q$  is not an approximation. This is the *very expression of the CLT*, rephrased using the Langevin equation and the justification for the characteristic function derivation.

We still have to solve the second equation in (29) to find the probability densities  $\rho(q)$ , but since we have the unknown (up to this point) function  $\Gamma_{22}(q)$  that depends upon  $q$  and that participates in this equation because of the term  $p(t)$ , this cannot be done in the same straightforward manner as we have done with the variable  $p$ . In fact, this is exactly the point at which Quantum Mechanics enters.

The result (60) shows that, for each point  $q$  of the configuration space, the momentum probability distribution is of the Gaussian type—as we have already obtained

from other considerations regarding the Central Limit Theorem, or those of the previous section.

The similarities of the present derivation of (60) and those of the previous papers [1–3] are obvious, but we can bring them together as a means of making explicit the function  $\Gamma_{22}(q)$  and, thus, being capable of making real simulations of actual physical systems.

Let us compare the result (60) with the one we obtained in section two for the joint probability density of any quantum system. From such a comparison it becomes quite obvious that, to simulate the quantum mechanical results with the system of equations (29) we must make the identification

$$\Gamma_{22}(q) = \gamma(\overline{\delta p^2}) = -\frac{\gamma \hbar^2}{4m} \frac{\partial^2 \ln \rho(q)}{\partial q^2}; \quad \bar{p}(q; t) = \frac{\partial S(q)}{\partial q}, \tag{62}$$

where both  $\rho(q) = R^2(q)$  and  $S(q)$  come from the solution of the Schrödinger equation with

$$\psi(q) = R(q) \exp\left(\frac{iS(q)}{\hbar}\right). \tag{63}$$

Because of these identifications, the first Langevin equation becomes an expression in which the mean-square deviation of  $p$ , given by

$$\sqrt{[\overline{\delta p(q, t)}]^2} = \sqrt{-\frac{\hbar^2}{4m} \frac{\partial^2 \ln \rho(q)}{\partial q^2}}, \tag{64}$$

enters as a *true* random force, because of the  $\xi_\ell$ . Thus, the relation with the Bohmian “quantum potential” becomes clear: Bohm’s equation is an equation for *average values* (such as  $\bar{p}(q, t)$ ) and the “quantum potential” does not appear as a true random force.

In the next section we present the result of simulations of the Langevin equations to two concrete physical systems: the one dimensional Harmonic Oscillator and the one dimensional Morse potential. We also show, for the Harmonic Oscillator example, the relation between the results of the simulation of the Langevin equations (29) and Bohm’s equation.

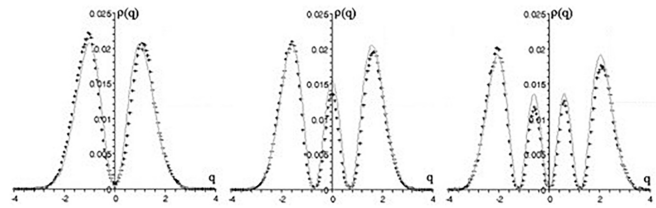
## 4. Examples

Langevin equations are quite easy to computationally simulate. We then present, in what follows, some results regarding concrete quantum mechanical systems just as a means to show the adequacy of the approach. The reader interested in the various details of these simulations should see [18, 23].

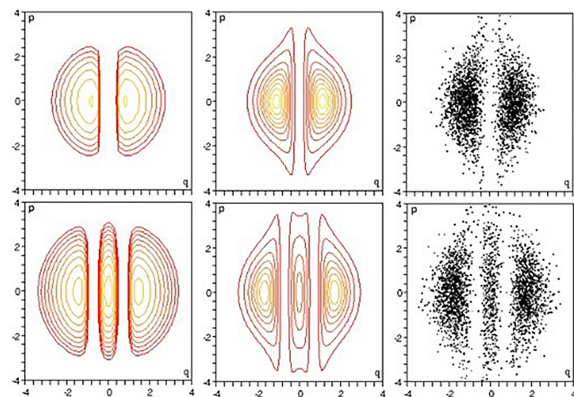
### 4.1. The Harmonic Oscillator

The quantum mechanical problem is defined by the potential

$$V(q) = \frac{1}{2} m \omega^2 q^2, \tag{65}$$



**Figure 2:** The results for the probability density function on configuration space for the Harmonic Oscillator problem for the first three excited states  $n = 1, 2, 3$ . The continuous curve is the theoretical one coming from the solution of the Schrödinger equation.



**Figure 3:** Comparison between Bohm’s trajectory for constant energy, equal probability curves of the phase space probability density function and the filling of the phase space made by simulating the corresponding Langevin equations.

with probability amplitudes given by

$$\psi(q) = \left(\frac{m\omega}{\hbar\pi^2}\right)^{1/4} \frac{1}{\sqrt{n!2^n}} \exp\left(\frac{-m\omega q^2}{2\hbar}\right) H_n\left(\sqrt{\frac{m\omega}{\hbar}}q\right), \tag{66}$$

where  $H_n$  is the Hermite polynomial. We make  $m = \hbar = \omega = 1$  and perform the computational simulations to get the results shown in Figure 2.

These simulations were made considering a *single particle* system randomly moving on phase space. One can also make the *ensemble simulation* of these equations to get equivalent results. We also can plot a comparison between the same energy curves coming from Bohm’s potential, the equal probability curves coming from the phase space probability density function, as we made in paper II, but now compared with the filling of the phase space coming from the dynamical Langevin equations. The result is shown in Figure 3 for the first two excited states of the Harmonic Oscillator.

### 4.2. The Morse Oscillator

For the quantum mechanical problem of the Morse Oscillator, we have the potential function

$$V(q) = \frac{D}{2} [\exp(-\beta(q - q_0)) - 1]^2, \tag{67}$$



with wave functions given by

$$\psi_n(y) = e^{-\sqrt{D}y} (2\sqrt{D}y)^{n-\sqrt{D}+1/2} L_n^{2n+1-2\sqrt{D}} (2\sqrt{D}y), \tag{68}$$

where  $q = 2\sqrt{D}y$  and  $L_n^m(q)$  are the Laguerre associated functions. We made our *single system* simulations for  $D = 16$  and for the quantum numbers  $n = 4, 5, 6, 7$  whose states are represented in Figure 4 (note that the last state is very close to the line of positive energy, meaning that it is easy for it to spontaneously ionize).

The probability density functions upon configuration space are shown in Figure 5 and show a very good fit to the theoretical ones.

These simulations are but a few examples. The reader can simulate the Langevin equations of Quantum Mechanics for whatever physical system of interest.

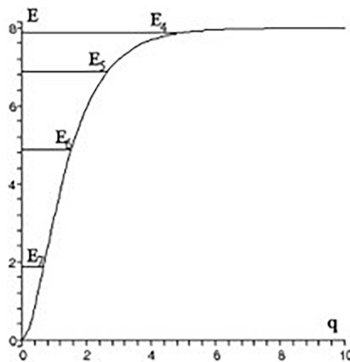


Figure 4: Energy states of the Morse Oscillator with  $D = 16$ .

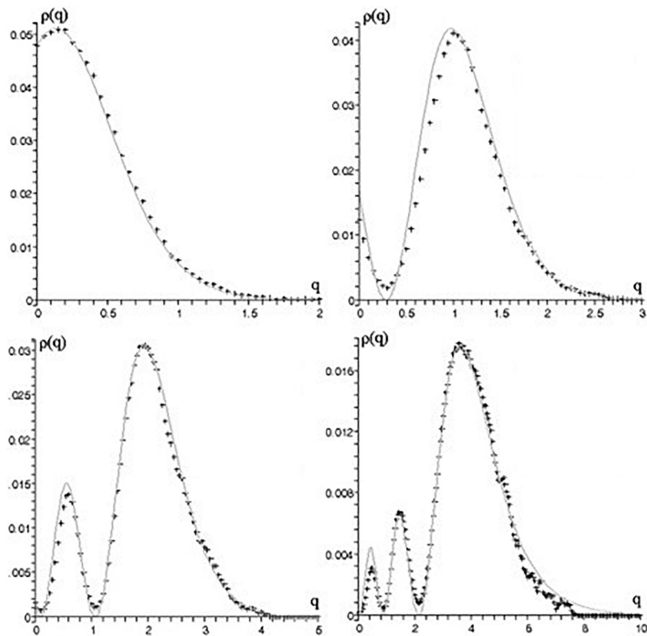


Figure 5: Probability density functions in configuration space for four levels of the Morse oscillator with  $D = 16$ . The continuous line is the theoretical curve coming from the solution of the Schrödinger equation.

### 5. Final Considerations

In paper III [3] we end the paper regretting that we had proved the Central Limit Theorem, but we did that without having any clue of the process by which the sum of random variables were performed, nor where they come from.

The approach using the Langevin equations to show that they reproduce all the results of Quantum Mechanics shows that these Langevin equations are the source of these random variables and sums of them.

In the process to show that, we needed to look “inside” the characteristic function, as defined together with the series of random variables, which brought us quite close to the mathematical techniques used to demonstrate that the Central Limit Theorem is a crucial part of the Quantum Mechanical formalism.

This paper, thus, connects the previous derivations of the Schrödinger equation to the stochastic one and we now have our demonstration scheme as shown in Figure 6.

Finding the Langevin equations for Quantum Mechanics gives the theory a *structure* similar to its classical counterpart. In Classical Mechanics we have *two* definitions for the state of a Newtonian system: the point-like phase space pair of coordinates  $(q(t), p(t))$  and the statistical phase space probability density function, given by  $F(q, p, t)$  and satisfying the Liouville theorem. If we find a Langevin equation for Quantum Mechanics, we will also have a point-like phase space pair of coordinates  $(q(t), p(t))$  for each realization of the quantum mechanical system, and a phase-space probability density function, given by  $F(q, p, t)$  defined to the quantum realm.

We then come to the end of our journey into (some) derivations of the Schrödinger equation. The attentive reader may then ask if the approach is able to derive the *relativistic* extension of the theory, based on the Klein-Gordon equation. To this question we *must* answer in

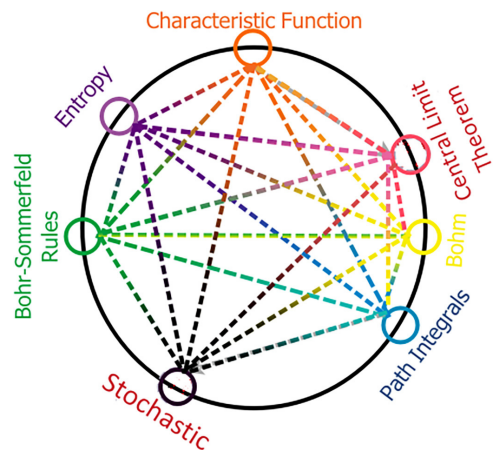


Figure 6: State of the art regarding derivations of the Schrödinger equation.



the affirmative, since there is no option for an axiomatic approach. Another possible extension of the approach would be the attempt to encompass non Hamiltonian forces, such as those related to dissipative forces. In future papers we will show that both these extensions come naturally from the derivations we have made so far.

Pointing to didactic extensions, we reinforce the relevance of absorb the type of discussion in this paper for teaching Quantum Mechanics in undergraduate and postgraduate courses. Alternative formulations, which nevertheless preserve in-depth understanding of a theory essential to the understanding of contemporary physics, are decidedly fundamental in processes of didactic transposition. These ventures that favor teaching in a critical, careful and creative way, aiming at meaningful learning, are fundamental to fields of knowledge that are still rare in curricula and teaching materials and that integrate considerable theoretical and mathematical abstractions. Similar efforts were made in discussions such as those found in previous papers [1–3, 24–31], which are complementary and illustrative of the didactic interest expressed here.

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## Supplementary Material

The following online material is available for this article: Supplementary material – Maple program to study the Langevin Equation for the Harmonic Oscillator problem.

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