The classical mechanics from the quantum equation

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ABSTRACT

This work shows that the stochastic generalization of the quantum hydrodynamic analogy (QHA) has its corresponding stochastic Schrödinger equation (SSE) as happens for the deterministic limit. The analysis shows that in presence of spatially distributed noise the quantum behavior is maintained on a distance shorter than the correlation length (λ_C) of fluctuations of the modulus of the wave function and that the SSE comprehends the standard one when λ_C tends to infinity respect to the scale of the problem.

The model shows that the term responsible of the non-local interaction into the Schrödinger equation may have a finite range of efficacy maintaining its non-local effect on a finite distance λ_L ("quantum non-locality length"). In the case, when the classical limit is approached, the model shows that the dynamics can be described by a non-linear SSE at the glance with the current theoretical outputs. In particular, the work shows that the semi-empirical Gross-Pitaevskii equation can be derived by the SSE.

Keywords: Quantum hydrodynamic analogy, quantum to classical transition; quantum decoherence; quantum dissipation; noise suppression; open quantum systems; quantum dispersive phenomena; quantum irreversibility

1. INTRODUCTION

The emergence of classical behavior from a quantum system is a problem of interest in many branches of physics. The incompatibility between the quantum and classical mechanics comes mainly from the non local character of the quantum mechanics. From the empirical point of view, it is widely accepted that fluctuations may destroy quantum coherence and elicit the emergence of the classical behavior. By using the alternative approach of the quantum hydrodynamic analogy (QHA) [1] in this paper we investigate how the fluctuations influence the quantum non locality and possibly lead to the large-scale classical evolution.

The motivation of using the QHA relies in the fact that it owns a classical-like structure that makes it suitable for the achievement of a comprehensive understanding of quantum and classical phenomena. The suitability of the classical-like theories in explaining open quantum phenomena is a matter of fact and is confirmed by their success in the description of the

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dispersive effects in semiconductors, multiple tunneling, mesocopic and quantum Brownian oscillators, critical phenomena, stochastic Bose-Einstain condensation and in the theoretical regularization procedure of quantum field [2-12]. The interest for the QHA had never interrupted, resulting useful in the numerical solution of the time-dependent Schrödinger equation [13] and had led to a number of papers and textbooks bringing original contributions to the comprehension of quantum dynamics [14-17]. The problems to which the QHA well applies are those whose scale is larger than that one of small atoms such as chromophore-protein complexes and semi-conducting polymers that are dynamically submitted to environmental fluctuations.

Compared to others classical-like approaches (e.g., the stochastic quantization procedure of Nelson [18] and the mechanics given by Bohm [19]) the QHA has the precious property to be exactly equivalent to the Schrödinger equation and to be free from problems such as the undefined variables of the Bohmian mechanics or the unclear relation between the statistical and the quantum fluctuations as in the Nelson theory. As clearly shown by Tsekov [20], it must be noted that the QHA has not to be confused with the Bohmian mechanics that is more like a mean-field limit of quantum mechanics.

Among the researches to which the present work has useful connections there are: The clarification of the hierarchy between the classical and quantum mechanics [18-20]; the description of mesoscopic system showing quantum-to classical transition [12]; the interplay between fluctuations and quantum coherence [21-25], The achievement of a consistent theory of quantum gravity [10]; The quantum treatment of chaos and irreversibility [21].

2. THEORY: THE SQHA EQUATION OF MOTION

When the noise is a stochastic function of the space, in the quantum hydrodynamic analogy the motion equation is described by the stochastic partial differential equation (SPDE) for the spatial density of number of particles n (i.e., the wave function modulus squared (WFMS)), that reads [26]

$$\partial_t \mathrm{n}_{(q,t)} = -\nabla_q \bullet (\mathrm{n}_{(q,t)} \dot{q}) + \eta_{(q,t,\Theta)} \qquad (1)$$

$$\dot{p} = -\nabla_q (V_{(q)} + V_{qu(\mathrm{n})}), \qquad (2)$$

$$\dot{q} = \frac{\nabla_q S}{m} = \frac{p}{m}, \qquad (3)$$

$$S = \int_{t_0}^{t} dt \left(\frac{p \bullet p}{2m} - V_{(q)} - V_{qu(\mathrm{n})} \right) \qquad (4)$$

where Θ is the amplitude of the spatially distributed noise η whose covariance matrix reads

$$< \eta_{(q_\alpha)}, \eta_{(q_\beta + \lambda)} > = < \eta_{(q_\alpha)}, \eta_{(q_\alpha)} > G(\lambda) \delta_{\alpha\beta} \qquad (5)$$

where $G(\lambda)$ is the dimensionless shape of the correlation function of the noise. Moreover, $V_{(q)}$ represents the Hamiltonian potential and $V_{qu(\mathrm{n})}$, the so called (non-local) quantum potential [14], that reads

$$V_{qu} = -\left(\frac{\hbar^2}{2m}\right) \mathrm{n}^{-1/2} \nabla_q \bullet \nabla_q \mathrm{n}^{1/2}$$

Close to the quantum deterministic limit the WFMS can be developed in a series of approximation $n \cong n_0 + \Delta n_1 + \Delta n_2 + \ldots + \Delta n_n$, where n_0 is the solution of the deterministic limit [26]. The condition that the fluctuations of the quantum potential $V_{qu(n)}$ do not diverge, as Θ goes to zero (so that the deterministic limit can be warranted) is implemented by operating on the system of the discrete version of the SPDE (1) whose variable reads

$$Y_i = \iiint_{\Delta_i} d^{3n}q \; n_{(q,t)}, \tag{6}$$

where the space hyper-cell $\Delta_i = [(\mathbf{q}_{(i-1)}, (\mathbf{q}_{(i)})]$ (with $\mathbf{q}_{(i)} - \mathbf{q}_{(i-1)} = \lambda$) is taken around the discrete point $q_{(\mathbf{i})}$.

In the limit of small Θ, the quantum potential fluctuations can be derived as a function of the fluctuations of the WFMS at the smallest order $n_0 + \Delta n_1$. The results show that, in order to have the quantum potential energy finite in the fluctuating state, i.e., $\lim_{\lambda \to 0} < V_{qu}, V_{qu} >$ finite, the following conditions must be fulfilled

$$\lim_{\lambda \to 0} \sum_{\alpha} \lambda^{-2} [1 - G_{(\lambda)}] < \infty \tag{7}$$

$$\lim_{\lambda \to 0} \sum_{\alpha} \lambda^{-4} [1 - G_{(\lambda)}]^2 < \infty \tag{8}$$

$$\lim_{\lambda \to 0} \sum_{\alpha} \lambda^{-4} [3 + G_{(2\lambda)} - 4G_{(\lambda)}] < \infty \tag{9}$$

Relations (7-9) can be easily understood observing that the quantum potential owns a membrane elastic-like behavior where a higher curvature of the WFMS leads to higher energy. The fact that white fluctuations of the WFMS brings to a zero curvature wrinkles of the WFMS (and hence to an infinite quantum potential energy) does not allow the realization of such a condition. The fact that independent fluctuations on smaller and smaller distance are progressively suppressed, means that exists a characteristic distance (let's name λ_c) above which the WFMS fluctuations are restrained in order to maintain the system energy finite.

Developing $G_{(\lambda)}$ in series expansion (for small Θ) as a function of $\frac{\lambda}{\lambda_c}$, where λ_c is analytically defined further on, conditions (7-9) leads to

$$\lim_{\lambda \to 0} G_{(\lambda)} \cong 1 \pm \left(\frac{\lambda}{\lambda_c}\right)^2 + a_4 \left(\frac{\lambda}{\lambda_c}\right)^4 + \sum_{j=5}^{\infty} a_j \left(\frac{\lambda}{\lambda_c}\right)^j . \tag{10}$$

where without a leaking of generality has been put $a_2 = \pm 1$ by a re-definition of the spatial cell side λ such as $\lambda' = a_2^{1/2} \lambda$.

In order to obtain a model coherent with (10), holding also for a large-scale approach, the shape of the correlation function can be assumed of the form

$$G_{(\lambda)} = exp[-(\frac{\lambda}{\lambda_c})^2] . \tag{11}$$

($a_2 = 1$ does not warrant the ergodicity). Thence, from (5) we obtain

$$< \eta_{(q_\alpha ,t)}, \eta_{(q_\beta + \lambda, t+\tau)} >= \underline{\mu} \frac{8m(k\Theta)^2}{\pi^3 \hbar^2} exp[-(\frac{\lambda}{\lambda_c})^2] \delta(\tau) \delta_{\alpha\beta} \tag{12}$$

where [26]

$$\lambda_c = (\frac{\pi}{2})^{3/2} \frac{\hbar}{(2mk\Theta)^{1/2}} \tag{13}$$

and where $\underline{\mu}$ is the WFMS mobility form factor that depends by specificity of the considered system [26].

2.1 Quantum non-locality length λ_L

In addition to the noise correlation function (11), to obtain the large-scale form of equations (1-5) we need to investigate the importance of the quantum force $\dot{p}_{qu} = -\nabla_q V_{qu}$ in (2) in the large-distance limit.
As shown in reference [26] the relevance of the force generated by the quantum potential (i.e., $|\nabla_q V_{qu}|$) at large distance can be evaluated by the convergence of the integral

$$\int_0^\infty | q^{-1} \nabla_q V_{qu} | dq \tag{14}$$

If the quantum potential force grows less than a constant at large distance so that $\lim_{|q| \to \infty} | q^{-1} \nabla_q V_{qu} | \propto | q |^{-(1+\varepsilon)}$, where $\varepsilon > 0$, the integral (14) converges. In this case, the quantum potential range of interaction can be evaluated by the mean weighted distance

$$\lambda_L = 2 \frac{\int_0^\infty | q^{-1} \frac{dV_{qu}}{dq} | dq}{\lambda_c^{-1} | \frac{dV_{qu}}{dq} |_{(q=\lambda_c)}} . \tag{15}$$

It is worth noting that for Gaussian-type states (as for linear systems) owing a quadratic quantum potential, so that it holds

$$\lim_{|q| \to \infty} | q^{-1} \nabla_q V_{qu} | = Constant$$

λ_L results infinite. In this case, the quantum non-local behavior is also effective on the large scale dynamics.

2.2 Schrödinger equation from the SQHA

For $\Theta = 0$ equation (1-3), with the identities

$$\dot{q} = \frac{\nabla_q S}{m} \qquad (16)$$

where

$$S = \int_{t_0}^{t} dt\left(\frac{p \bullet p}{2m} - V_{(q)} - V_{qu} \right) \qquad (17)$$

and

$$\mathrm{n}_{(q,t)} = A^2_{(q,t)} \qquad (18)$$

can be derived [27] by the system of two coupled differential equations that read

$$\partial_t S_{(q,t)} = -V_{(q)} + \frac{\hbar^2}{2m} \frac{\nabla_q{}^2 A_{(q,t)}}{A_{(q,t)}} - \frac{1}{2m}\left(\nabla_q S_{(q,t)} \right)^2 \qquad (19)$$

$$\partial_t A_{(q,t)} = -\frac{1}{m} \nabla_q A_{(q,t)} \bullet \nabla_q S_{(q,t)} - \frac{1}{2m} A \nabla_q{}^2 S_{(q,t)} \qquad (20)$$

that for the complex variable

$$\psi_{(q,t)} = A_{(q,t)} \exp\left[\frac{\mathrm{i}}{\hbar} S_{(q,t)} \right] \qquad (21)$$

is equivalent to set to zero the real and imaginary part of the Schrödinger equation

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla_q{}^2 \psi + V_{(q)} \psi \, . \qquad (22)$$

For $\Theta \neq 0$ the stochastic equations (1-3) can be obtained by the following system of differential equations

$$\partial_t S_{(q,t)} = -V_{(q)} + \frac{\hbar^2}{2m} \frac{\nabla_q{}^2 A_{(q,t)}}{A_{(q,t)}} - \frac{1}{2m}\left(\nabla_q S_{(q,t)} \right)^2 \qquad (23)$$

$$\partial_t A_{(q,t)} = -\frac{1}{m} \nabla_q A_{(q,t)} \bullet \nabla_q S_{(q,t)} - \frac{1}{2m} A \nabla_q{}^2 S_{(q,t)} + A^{-1} \eta_{(q_\alpha, t, \Theta)} \qquad (24)$$

that for the complex variable (21) are equivalent to the SSE

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\nabla_q{}^2\psi+V_{(q)}\psi+i\frac{\psi}{|\psi|^2}\eta_{(q_\alpha,t,\Theta)}. \tag{25}$$

2.3 Limiting dynamics

Generally speaking, given a problem with a physical length ΔL, depending by the two lengths λ_c and λ_L, built-in into the SQHA, various limiting dynamics follow:

1) *Non-local deterministic dynamics* (i.e., standard quantum mechanics) with $\Delta L << \lambda_c \cup \lambda_L$ (e.g., $\Theta \to 0$). In this case the deterministic QHA and the Schrödinger equation (22) are obtained since

$$<\eta_{(q_\alpha,t)},\eta_{(q_\alpha+\lambda,t+\tau)}>=0 \tag{26}$$

2) *Non-local quantum-stochastic dynamics*, with $\lambda_c << \Delta L << \lambda_L$

In this case the noise correlation function reads

$$<\eta_{(q_\alpha,t)},\eta_{(q_\alpha+\lambda,t+\tau)}>=\underline{\mu}\,\delta_{\alpha\beta}\frac{2k\Theta}{\lambda_c}\delta(\lambda)\delta(\tau) \tag{27}$$

3) *Local stochastic dynamics*, with $\lambda_c \cup \lambda_L << \Delta L$.

Given the condition $\lambda_L << \Delta L$ so that it holds

$$\lim_{|q|\to\infty}|\nabla_q V_{qu(n_0)}|=0 \tag{28}$$

the SPDE of motion acquires the form

$$\partial_t n_{(q,t)}=-\nabla_q\bullet(n_{(q,t)}\dot{q})+\eta_{(q_\alpha,t,\Theta)} \tag{29}$$

with $<\eta_{(q_\alpha,t)},\eta_{(q_\alpha+\lambda,t+\tau)}>$ given by (27) and

$$\dot{q}=\frac{p}{m}=\nabla_q\lim_{\Delta L/\lambda_L\to\infty}\frac{\nabla_q S}{m}=\nabla_q\{\lim_{\Delta L/\lambda_L\to 0}\frac{1}{m}\int_{t_0}^{t}dt(\frac{p\bullet p}{2m}-V_{(q)}-V_{qu(n)}-I^*)\}$$

$$=\frac{1}{m}\nabla_q\{\int_{t_0}^{t}dt\,(\frac{p\bullet p}{2m}-V_{(q)}-\Delta)\}=\frac{p_{cl}}{m}+\frac{\delta p}{m}\cong\frac{p_{cl}}{m} \tag{30}$$

where δp is a small fluctuation of the momentum and

$$\dot{p}_{cl}=-\nabla_q V_{(q)}. \tag{31}$$

In this case, by using the identities (16-18) we can write

$$\partial_t \mathrm{S} = -V_{(q)} - \frac{1}{2m}(\nabla_q \mathrm{S})^2 \qquad (32)$$

$$\partial_t A_{(q,t)} = -\frac{1}{m}\nabla_q A_{(q,t)} \bullet \nabla_q S_{(q,t)} - \frac{1}{2m} A \nabla_q{}^2 S_{(q,t)} + A^{-1}\eta_{(q_\alpha,t,\Theta)} \qquad (33)$$

Clearly, it is not possible to obtain the Schrödinger equation by (32-33) since S given by (30) converges to the classical value S_{cl}

$$S_{cl} = \int_{t_0}^{t} dt\,(\frac{p \bullet p}{2m} - V_{(q)}). \qquad (34)$$

Nevertheless, for the wave function $\psi_{(q,t)}$ the classically stochastic equations of motion (32-33) can be cast in a non-linear Schrödinger equation (NLSE) that reads:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}(\nabla_q{}^2\psi - \frac{\psi}{|\psi|}\nabla_q{}^2|\psi|) + V_{(q)}\psi + i\frac{\psi}{|\psi|^2}\eta_{(q_\alpha,t,\Theta)}. \qquad (35)$$

The former differential equation describes the evolution of a WFMS owing a classical action S_{cl}. Actually, the exact equation is given by (25) while the former one (35) is just a limiting one and the formal transformation between them is just intrinsic.

Alternatively, in order to describe phenomena at the edge between the classical and the quantum behavior, a semi-empirical equation for passing from (25) to (35) could be more manageable.

By considering that the when the physical length of the system $\Delta\mathrm{L}$ is much smaller than the quantum non-locality length λ_L, the system is quantum, while when λ_L is very small compared to $\Delta\mathrm{L}$ is classic, it is possible to write

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}(\nabla_q{}^2\psi - \alpha\frac{\psi}{|\psi|}\nabla_q{}^2|\psi|) + V_{(q)}\psi + i\frac{\psi}{|\psi|^2}\eta_{(q_\alpha,t,\Theta)} \qquad (36)$$

where α (a dimensionless quantum-to-classical parameter) at first order in a series expansion as a function of the ratio $\frac{\lambda_L}{\Delta\mathrm{L}}$, reads

$$\alpha \cong \frac{\frac{\Delta\mathrm{L}}{\lambda_L}}{1+\frac{\Delta\mathrm{L}}{\lambda_L}} \qquad (37)$$

In the case when (36) is used to describe a system at the boundary between the quantum and the classical dynamics (i.e., $\frac{\lambda_L}{\Delta L} \approx 1$) we have $\alpha \approx \frac{1}{2}$.

It is interesting to note that Equation (36) for pseudo-Gaussian states that have the large-distance hyperbolic behavior

$$\lim_{|q| \to \infty} |\psi| \propto a^{-1/2} q^{-1} \tag{38}$$

that holds for Lennard-Jones type potentials

$$V_{L-J(q)} = 4V_0 [(\frac{\sigma}{r})^{12} - (\frac{\sigma}{r})^{6}] \tag{39}$$

such as in the ^{4}He dimer [28], equation (36) acquires the stochastic form of the Gross-Pitaevskii one [29]

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} (\nabla_q{}^2 \psi - \frac{a}{4} |\psi|^2 \psi) + V_{(q)} \psi + i \frac{\psi}{|\psi|^2} \eta_{(q_\alpha, t, \Theta)} \tag{40}$$

3. DISCUSSION AND CONCLUSIONS

Being $\eta_{(q_\alpha, t, \Theta)}$ a random process with a finite correlation distance λ_c, when the physical length of the problem is much smaller than it, (25) converges to the standard Schrödinger equation comprehending it.

The stochastic generalization (25) is able to describe the classical states since, in non-linear (weakly bonded) systems, the term $\frac{\psi}{|\psi|} \nabla_q{}^2 |\psi|$ (that brings the non-local quantum interaction) may become negligibly small in problems whose scale is much larger than its interaction distance λ_L. The following large-scale limiting classical dynamics is described by the NLSE (35).

The approximated NLSE describing dynamics near the quantum-to-classical transition (36), where the non-local quantum interaction term is progressively subtracted (by the factor α) for hyperbolic large-distance wave function, such as that one of the ^{4}He dimer, leads to the Gross-Pitaevskii equation that is well experimentally verified.

From the general point of view the SSE (25) can be helpful in describing at larger extent open quantum systems where the environmental fluctuations and the classical effects start to be relevant.

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NOMENCLATURE

n : squared wave function modulus	l^{-3}
S : action of the system	m^{-1} l^{-2} t
m : mass of structureless particles	m
$\hbar$: Plank’s constant	m l^{2} t^{-1}
c : light speed	l t^{-1}
k : Boltzmann’s constant	m l^{2} t^{-2}/°K
Θ : Noise amplitude	°K
H : Hamiltonian of the system	m l^{2} t^{-2}
V : potential energy	m l^{2} t^{-2}
V_{qu} : quantum potential energy	m l^{2} t^{-2}
η : Gaussian noise of WFMS	l^{-3} t^{-1}
λ_c : correlation length of squared wave function modulus fluctuations	l
λ_L : range of interaction of non-local quantum interaction	l
G(λ) : dimensionless correlation function (shape) of WFMS fluctuations	pure number
$\underline{\mu}$: WFMS mobility form factor	m^{-1} t l^{-6}
μ = WFMS mobility constant	m^{-1} t