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 similarly happens for the deterministic limit. The SSE owns an imaginary random noise that has a finite correlation distance, so that when the physical length of the problem is much smaller than it, the SSE converges to the standard Schrödinger equation comprehending it. The model shows that in non-linear (weakly bounded) systems, the term responsible of the non-local interaction in the SSE may have a finite range of efficacy maintaining its non-local effect on a finite distance. A non-linear SSE that describes the related large-scale classical dynamics is derived. The work also shows that at the edge between the quantum and the classical regime the SSE can lead to the semi-empirical Gross-Pitaevskii equation.

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

1. INTRODUCTION

By using the stochastic generalization of the quantum hydrodynamic analogy (QHA) [1-2] that describes how fluctuations influence the quantum non-locality and possibly lead to the large-scale classical evolution, we derive here the corresponding stochastic Schrödinger equation (SSE) able to describe the classical to quantum transition and to lead to the classical evolution.

The motivation of using the QHA approach to derive the SSE relies in the fact that it owns a classical-like structure that allows the achievement of a comprehensive understanding of quantum and classical phenomena. The QHA well applies to problems whose scale is larger than that one of small atoms, which are dynamically submitted to environmental fluctuations. This is confirmed by its success in the description of chromophore-protein complexes and semi-conducting polymers, dispersive effects in semiconductors, multiple tunneling, mesocopic and quantum Brownian oscillators, critical phenomena, stochastic Bose-Einstein condensation and in the theoretical regularization procedure of quantum field [3-13]. The QHA has resulted useful in the numerical solution of the time-dependent Schrödinger

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equation [14] and has led to a number of papers and textbooks bringing original contributions to the comprehension of quantum dynamics [15-18]. Compared to others classical-like approaches (e.g., the stochastic quantization procedure of Nelson [19] and the mechanics given by Bohm [20]) the QHA owns a well defined correspondence with the Schrödinger equation and is free from problems such as the undefined variables of the Bohmian mechanics [21] or the unclear relation between the statistical and the quantum fluctuations as in the Nelson theory.

The present work brings the unitary description of the stochastic quantum hydrodynamic analogy (SQHA) into the Schrödinger approach. The derived SSE owns a theoretical connection with the classical non-linear Schrödinger equation and the Gross-Pitaevskii one showing to be usefully applicable to the problems of quantum-to-classical transition [13], quantum de-coherence [22-26] and quantum treatment of chaos and irreversibility [22].

2. THEORY: THE SQHA EQUATION OF MOTION

When the noise is a stochastic function of the space, in the SQHA 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 [2]

$$\partial_t n_{(q,t)} = -\nabla_q \bullet (n_{(q,t)} \dot{q}) + \eta_{(q,t,\Theta)} \tag{1}$$

$$< \eta_{(q_\alpha)}, \eta_{(q_\beta + \lambda)} > = < \eta_{(q_\alpha)}, \eta_{(q_\alpha)} > G(\lambda) \delta_{\alpha\beta} \tag{2}$$

$$\dot{p} = -\nabla_q (V_{(q)} + V_{qu(n)}), \tag{3}$$

$$\dot{q} = \frac{\nabla_q S}{m} = \frac{p}{m}, \tag{4}$$

$$S = \int_{t_0}^{t} dt(\frac{p \bullet p}{2m} - V_{(q)} - V_{qu(n)}) \tag{5}$$

where Θ is the amplitude of the spatially distributed noise η, $V_{(q)}$ represents the Hamiltonian potential and $V_{qu(n)}$ is the so-called (non-local) quantum potential [15] that reads

$$V_{qu} = -(\frac{\hbar^2}{2m}) n^{-1/2} \nabla_q \bullet \nabla_q n^{1/2}. \quad . \tag{6}$$

Moreover, $G(\lambda)$ is the dimensionless shape of the correlation function of the noise η.

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) leads to a $G(\lambda)$ owing the form [2]

$$G(\lambda) = exp[-(\frac{\lambda}{\lambda_c})^2] . \tag{7}$$

This result is a direct consequence of the quantum potential form that owns a membrane elastic-like energy where a higher curvature of the WFMS leads to higher energy. White fluctuations of the WFMS that bring to a zero curvature wrinkles of the WFMS (and hence to an infinite quantum potential energy) are not allowed. The fact that, in order to maintain the system energy finite, independent fluctuations on smaller and smaller distance are progressively suppressed, leads (in the small noise limit) to the existence of a correlation distance (let's name it λ_c) for the noise.

Thence, (2) reads [2]

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

where

$$\lambda_c=(\frac{\pi}{2})^{3/2}\frac{\hbar}{(2mk\Theta)^{1/2}} \qquad (9)$$

and where $\underline{\mu}$ is the WFMS mobility form factor that depends by the specificity of the considered system [2].

2.2 Schrödinger equation from the SQHA

For $\Theta = 0$ equations (1-5), with the identities

$$\dot{q}=\frac{\nabla_q S}{m} \qquad (10)$$

where

$$S=\int_{t_0}^{t}dt(\frac{p\bullet p}{2m}-V_{(q)}-V_{qu}) \qquad (11)$$

and

$$\mathrm{n}_{(q,t)}=A^2_{(q,t)} \qquad (12)$$

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

$$\partial_t S_{(q,t)}=-V_{(q)}+\frac{\hbar^2}{2m}\frac{\nabla_q{}^2 A_{(q,t)}}{A_{(q,t)}}-\frac{1}{2m}(\nabla_q S_{(q,t)})^2 \qquad (13)$$

$$\partial_t A_{(q,t)}=-\frac{1}{m}\nabla_q A_{(q,t)}\bullet\nabla_q S_{(q,t)}-\frac{1}{2m}A\nabla_q{}^2 S_{(q,t)} \qquad (14)$$

that for the complex variable

$$\psi_{(q,t)}=A_{(q,t)}\exp[\frac{i}{\hbar}S_{(q,t)}] \qquad (15)$$

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

$$i\hbar\frac{\partial\psi}{\partial t}=-\frac{\hbar^2}{2m}\nabla_q{}^2\psi+V_{(q)}\psi\,. \qquad (16)$$

For $\Theta \neq 0$ the stochastic equations (1-5) can be obtained by the following system of differential equations

$$\partial_t S_{(q,t)} = -V_{(q)} + \frac{\hbar^2}{2m}\frac{\nabla_q{}^2 A_{(q,t)}}{A_{(q,t)}} - \frac{1}{2m}(\nabla_q S_{(q,t)})^2 \quad (17)$$

$$\partial_t A_{(q,t)} = -\frac{1}{m}\nabla_q A_{(q,t)} \bullet \nabla_q S_{(q,t)} - \frac{1}{2m} A \nabla_q{}^2 S_{(q,t)} + A^{-1}\eta_{(q_\alpha,t,\Theta)} \quad (18)$$

which for the complex variable (15) are equivalent to the SSE

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla_q{}^2\psi + V_{(q)}\psi + i\frac{\psi}{|\psi|^2}\eta_{(q_\alpha,t,\Theta)}. \quad (19)$$

2.3 Large-scale local non-linear Schrödinger equation

In addition to the noise correlation function (7), in the large-distance limit, it is also important to know the behavior of the quantum force $\dot{p}_{qu} = -\nabla_q V_{qu}$.

The relevance of the force generated by the quantum potential at large distance can be evaluated by the convergence of the integral [2]

$$\int_0^\infty | q^{-1}\nabla_q V_{qu} | dq \quad (20)$$

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 (20) converges. In this case, the mean weighted distance

$$\lambda_L = 2\frac{\int_0^\infty | q^{-1}\frac{dV_{qu}}{dq} | dq}{\lambda_c{}^{-1} | \frac{dV_{qu}}{dq} |_{(q=\lambda_c)}}, \quad (21)$$

can evaluate the quantum potential range of interaction.

Faster the Hamiltonian potential grows, more localized is the WFMS and hence stronger is the quantum potential. For the linear interaction, the Gaussian-type eigenstates leads to a quadratic quantum potential and, hence, to a linear quantum force, so that $\lim_{|q|\to\infty} | q^{-1}\nabla_q V_{qu} | \propto constant$ and λ_L diverges. Therefore, in order to have λ_L finite (so that the large-scale classical limit can be achieved) we have to deal with a system of particles interacting by a weaker than the linear interaction.

In the following, we derive local limiting dynamics for the SSE with $\lambda_c \cup \lambda_L << \Delta L$.

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

$$\lim_{|q|\to\infty} |\nabla_q V_{qu(\mathrm{n}_0)}| = 0 \tag{22}$$

and $\lambda_c << \Delta L$, by which (11) reads [2]

$$\begin{aligned}\dot{q} = \frac{p}{m} &= \lim_{\Delta L/\lambda_c\to 0}\ \lim_{\Delta L/\lambda_L\to\infty}\frac{\nabla_q S}{m} = \nabla_q\{\lim_{\Delta L/\lambda_c\to 0}\ \lim_{\Delta L/\lambda_L\to 0}\frac{1}{m}\int_{t_0}^{t} dt(\frac{p\bullet p}{2m} - V_{(q)} - V_{qu(\mathrm{n})})\}\\ &= \nabla_q\{\lim_{\Delta L/\lambda_c\to 0}\ \lim_{\Delta L/\lambda_L\to 0}\frac{1}{m}\int_{t_0}^{t} dt(\frac{p\bullet p}{2m} - V_{(q)} - V_{qu(\mathrm{n}_0)} - (V_{qu(\mathrm{n})} - V_{qu(\mathrm{n}_0)}))\}\\ &= \frac{1}{m}\nabla_q\{\int_{t_0}^{t} dt\,(\frac{p\bullet p}{2m} - V_{(q)} - \lim_{\Delta L/\lambda_c\to 0}(V_{qu(\mathrm{n})} - V_{qu(\mathrm{n}_0)}))\} = \frac{p_{cl}}{m} + \frac{\delta p}{m} \cong \frac{p_{cl}}{m}\end{aligned} \tag{23}$$

where, δp is a small fluctuation of the momentum, since

$$\lim_{\Delta L/\lambda_c\to 0}(V_{qu(\mathrm{n})} - V_{qu(\mathrm{n}_0)})) = \lim_{\Theta\to 0}\ (V_{qu(\mathrm{n})} - V_{qu(\mathrm{n}_0)})) = 0\,,$$

and

$$\dot{p}_{cl} = -\nabla_q V_{(q)}\,, \tag{24}$$

from (22) it follows that (18-19) read

$$\partial_t \mathrm{S} = -V_{(q)} - \frac{1}{2m}(\nabla_q \mathrm{S})^2 \tag{25}$$

$$\partial_t A_{(q,t)} = -\frac{1}{m}\nabla_q A_{(q,t)} \bullet \nabla_q S_{(q,t)} - \frac{1}{2m}A\nabla_q{}^2 S_{(q,t)} + A^{-1}\eta_{(q_\alpha,t,\Theta)} \tag{26}$$

Where S given by (23) converges to the classical value S_{cl} and where

$$\lim_{\Delta L/\lambda_c\to 0} <\eta_{(q_\alpha,t)},\eta_{(q_\alpha+\lambda,t+\tau)}> = \underline{\mu}\,\delta_{\alpha\beta}\frac{2k\Theta}{\lambda_c}\delta(\lambda)\delta(\tau) \tag{27}$$

For the wave function $\psi_{(q,t)}$ the classically stochastic equations of motion (25-26) can be cast in a non-linear Schrödinger equation (NLSE) that reads:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}(\nabla_q{}^2\psi - \frac{\psi}{|\psi|}\nabla_q{}^2|\psi|) + V_{(q)}\psi + i\frac{\psi}{|\psi|^2}\eta_{(q_\alpha,t,\Theta)}\,. \tag{28}$$

2.4 Semi-empirical non-linear Schrödinger equation for quantum-to-classical transition

Actually, the exact equation is given by (19) while the former one (28) is just a limiting one and the formal transformation between them is intrinsic.

Alternatively to (19), in order to describe phenomena at the edge between the classical and the quantum behavior, a semi-empirical equation for passing from (19) to (28) could be more manageable.

By considering that the when the physical length of the system ΔL is much smaller than the quantum non-locality length λ_L, the system is quantum, while when λ_L is very small compared to ΔL is classic, it is possible to write

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\nabla_q{}^2 \psi - \alpha \frac{\psi}{|\psi|}\nabla_q{}^2 |\psi|\right) + V_{(q)}\psi + i\frac{\psi}{|\psi|^2}\eta_{(q_\alpha,t,\Theta)} \qquad (29)$$

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

$$\alpha \cong \frac{\frac{\Delta L}{\lambda_L}}{1+\frac{\Delta L}{\lambda_L}} \qquad (30)$$

In the case when (29) 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 (29) for pseudo-Gaussian states that have the large-distance hyperbolic behavior

$$\lim_{|q|\to\infty} |\psi| \propto a^{-1/2} q^{-1} \qquad (31)$$

that holds for Lennard-Jones type potentials

$$V_{L-J(q)} = 4V_0\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \qquad (32)$$

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

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\left(\nabla_q{}^2 \psi - \frac{a}{4}|\psi|^2 \psi\right) + V_{(q)}\psi + i\frac{\psi}{|\psi|^2}\eta_{(q_\alpha,t,\Theta)} \qquad (33)$$

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, (19) converges to the standard Schrödinger equation comprehending it.

The stochastic generalization (19) is able to describe the classical states since, in non-linear (weakly bounded) 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 (28).

The approximated NLSE describing dynamics near the quantum-to-classical transition (29), 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 (19) 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	$m^{-1}\ t$