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TITLE: QUANTUM DIFFUSION

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AUTHOR(S): Salman Habib

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MASTER

Los Alamos

Los Alamos National Laboratory
Los Alamos, New Mexico 87545

Quantum Diffusion

Salman Habib

T-6, Theoretical Astrophysics

and

T-8, Elementary Particles and Field Theory

Los Alamos National Laboratory

Los Alamos, NM 87545

Abstract

We consider a simple quantum system subjected to a classical random force. Under certain conditions it is shown that the noise-averaged Wigner function of the system follows an integro-differential stochastic Liouville equation. In the simple case of polynomial noise-couplings this equation reduces to a generalized Fokker-Planck form. With nonlinear noise injection new “quantum diffusion” terms arise that have no counterpart in the classical case. Two special examples that are not of a Fokker-Planck form are discussed: the first with a localized noise source and the other with a spatially modulated noise source.

1. Stochastic Liouville Equations

Stochastic equations have long been used in physics to model various phenomena. Brownian motion, spin relaxation, and critical dynamics may be cited as obvious examples. At a formal level there are two ways to set up such equations (1) as *exact* equations [1][2] or (2) as part of a phenomenological description [3]. In either case one typically encounters equations that are nonlocal in time and involve stochastic forcing terms usually called “noise.” Such Langevin equations exist at both the classical and quantum levels. As expected the situation is more complicated in the latter case; while in classical problems it is often possible to approximate the “noise” as being Gaussian and white, and further to replace a nonlocal kernel by one local in time (the Markov approximation), such simplifications do not easily obtain in quantum mechanics. Nevertheless, simple approximate approaches are valuable in that they often capture some essential physics, or even make some technical point, with less calculational clutter when compared to a more comprehensive method of attack. The work outlined here is in this spirit. It owes much to Kubo’s work on the stochastic Liouville equation [4] and a presentation of it given by Zwanzig [5]. Different aspects

of this work have been considered in detail elsewhere [6]. Nonlinear couplings to an oscillator environment have been studied in the independent oscillator model in Ref. [7] where quantum diffusion has also been shown to exist.

In this paper, all quantum calculations will be done in the Wigner framework of quantum mechanics. Partly this is because quantum distribution functions defined on a mock phase space can be easily compared to their classical counterparts. Furthermore, in the models that will be discussed, stochastic Liouville equations written in terms of the Wigner function will be obtained directly from the stochastic Hamiltonian. This enables us to bypass the somewhat delicate question of how to derive quantum Fokker-Planck equations starting from Langevin equations for quantum operators. A nice feature of the phase space approach is that the quantum derivation of the stochastic Liouville equation closely parallels the classical derivation; there is no need to invoke path integrals. Finally, this approach also enables us to discuss the singular nature of the $\hbar \rightarrow 0$ limit for both the systematic and the diffusive terms in the stochastic Liouville equation.

We begin with the Hamiltonian (a generalization of the randomly forced oscillator considered earlier by Merzbacher [8]):

$$H = \frac{p^2}{2m} + V(x) - F(t)g(x), \quad (1)$$

where p, x are the dynamical variables characterizing the motion of the system. The functions $V(x)$ and $g(x)$ are assumed to be differentiable. $F(t)$ is an external perturbation that is taken to be Gaussian, white noise, *i.e.*, $\langle F(t) \rangle_N = 0$, and

$$\langle F(t_1)F(t_2) \rangle_N = 2B(t_1)\delta(t_1 - t_2), \quad (2)$$

with the usual restrictions on the higher moments. The $\langle \quad \rangle_N$ denotes an average over the realizations of F . The delta function in (2) is taken never to be exactly realized, but is treated just as an idealization of a sharply peaked, symmetric function. This corresponds to interpreting the noise in the sense of Stratonovich [9].

One way to write the equations of motion is to use the Liouville equation for the phase space distribution function. We introduce the distribution function $f(x, p; t)$, which satisfies the probability flux conservation equation (Liouville's theorem),

$$\frac{\partial}{\partial t} f(x, p; t) = -\frac{\partial}{\partial x} \left[\frac{\partial H}{\partial p} f(x, p; t) \right] - \frac{\partial}{\partial p} \left[-\frac{\partial H}{\partial x} f(x, p; t) \right], \quad (3)$$

the right hand side of (3) defining the Liouville operator L .

Following Kubo's analysis [4] applied to the Hamiltonian (1), we proceed to derive the noise-averaged stochastic Liouville equation. With L_0 the Liouville operator

corresponding to the systematic part of the evolution, we obtain.

$$\frac{\partial}{\partial t} \langle f(t) \rangle_N = -L_0 \langle f(t) \rangle_N + \left[B(t) \left(\frac{\partial g}{\partial x} \right)^2 \left(\frac{\partial^2}{\partial p^2} \right) \right] \langle f(t) \rangle_N. \quad (4)$$

a Fokker-Planck equation for the noise-averaged distribution function. Since f is a phase space distribution function, (4) is a two-variable Fokker-Planck, or Kramers, equation. In the absence of noise it reduces to the usual Liouville equation. We observe that whatever $V(x)$ and $g(x)$ may be, $\langle f(t) \rangle_N$ will *always* satisfy a Fokker-Planck equation. This will not be true in the quantum case, to which we now proceed.

As in the classical case we will work with the stochastic Hamiltonian (1). Because of the noise, this Hamiltonian will evolve pure states to mixed states. Thus it is appropriate to study not the time dependent Schrödinger equation but rather the quantum Liouville equation for the density matrix, given here in the coordinate representation,

$$i\hbar \frac{\partial}{\partial t} \rho(x_1, x_2) = [H(x_1) - H(x_2)^*] \rho(x_1, x_2). \quad (5)$$

We wish to write (5) in the Wigner formalism of quantum mechanics [10] and then to noise average just as in the classical case. This derivation is given in the first and third papers of Ref. [6] and here we quote only the final result:

$$\frac{\partial}{\partial t} \langle f_W(X, k; t) \rangle_N = -L_0 \langle f_W(X, k; t) \rangle_N - \int_{-\infty}^{+\infty} dp \langle f_W(X, k + p; t) \rangle_N K_S(X, p; t), \quad (6)$$

where

$$K_S(X, p; t) = \frac{B(t)}{\pi \hbar^3} \int_{-\infty}^{+\infty} dx e^{2ipx/\hbar} [g(X+x) - g(X-x)]^2 \quad (7)$$

and L_0 is the systematic quantum Liouville operator. When $g(X)$ can be profitably Taylor expanded, the above equation can be written as

$$\frac{\partial}{\partial t} \langle f_W(t) \rangle_N = -L_0 \langle f_W(t) \rangle_N + [B(t)L^2] \langle f_W(t) \rangle_N. \quad (8)$$

where

$$\begin{aligned} L^2 &= \left(\frac{\partial g}{\partial X} \right)^2 \frac{\partial^2}{\partial k^2} + 2 \left(\frac{\partial g}{\partial X} \right) \sum_{\lambda \text{ odd}} \frac{1}{\lambda!} \left(\frac{\hbar}{2i} \right)^{\lambda-1} \left(\frac{\partial^\lambda g}{\partial X^\lambda} \right) \frac{\partial^{\lambda+1}}{\partial k^{\lambda+1}} \\ &+ \sum_{\lambda, \nu \text{ odd}} \frac{1}{\lambda! \nu!} \left(\frac{\hbar}{2i} \right)^{\lambda+\nu-2} \left(\frac{\partial^\lambda g}{\partial X^\lambda} \right) \left(\frac{\partial^\nu g}{\partial X^\nu} \right) \frac{\partial^{\lambda+\nu}}{\partial k^{\lambda+\nu}}. \end{aligned} \quad (9)$$

2. Quantum Diffusion

The conditions under which (8) will reduce to a Fokker-Planck form are when both $V(X)$ and $g(X)$ are of the form $Ax + Bx^2$. In this case, $L_0 = 0$, and the quantum Liouville equation reduces to the classical one. The difference between the two cases

then lies not in the dynamical equation, but in the different constraints imposed on the initial value of the respective distribution functions.

We now study different choices for $g(X)$. If $g(X) = \Lambda X$, with Λ a constant, then $L^2 = \Lambda^2 \frac{\partial^2}{\partial k^2}$, a conventional diffusion term. This is the simple model equation often employed in studies of quantum decoherence [11].

Consider now the case, $g(X) = \Lambda X + \frac{1}{3}\epsilon X^3$, where

$$L^2 = (\Lambda + \epsilon X^2)^2 \frac{\partial^2}{\partial k^2} - \frac{1}{6}(\Lambda + \epsilon X^2)\epsilon \hbar^2 \frac{\partial^4}{\partial k^4} + \frac{1}{144}\epsilon^2 \hbar^4 \frac{\partial^6}{\partial k^6}. \quad (10)$$

Notice the appearance of the purely quantum mechanical, higher even derivative “diffusion” terms. The classical limit $\hbar \rightarrow 0$ is singular not only for the systematic quantum Liouville operator [12][13] but also for the stochastic terms arising from quantum diffusion. It is easy to see that all the quantum diffusive terms, when acting on “fast” (cf. Refs. [12][13]) pieces $\sim \exp(ikX/\hbar)$ of a Wigner function, are of $O(1/\hbar^2)$. The highest order quantum diffusion term dominates at large distances and always acts to increase the linear entropy $1 - \int dX dk f^2$ [6]. The effect of the quantum diffusion terms with regard to decoherence is to reduce the decoherence time at large length scales [6][7].

3. Two Illustrative Examples

As we have seen, the stochastic quantum Liouville equation written in terms of the Wigner distribution function is in general a complicated integro-differential equation. If the coupling to the noise is through a polynomial in the system variable, then this equation can truncate to a finite order partial differential equation. However, there are cases of physical interest where the coupling to the noise cannot be reduced to such a form. We will now exhibit two such cases, coupling the system (1) to a localized noise source, and (2) to a spatially modulated noise source. The first case is of interest in quantum tunneling through a stochastic barrier while the second applies to the noise in a microwave cavity. More details can be found in the third paper of Ref. [6].

A localized noise source can be modeled by setting $g(X) = \Lambda \exp(-\epsilon X^2/2)$. In this case,

$$\begin{aligned} \frac{\partial}{\partial t} \langle f_W(X, k; t) \rangle_N &= -L_{S_{y_0}} \langle f_W(X, k; t) \rangle_N - \frac{2B\Lambda^2}{\text{sgn}t \epsilon \pi \hbar^3} \int_{-\infty}^{+\infty} dp \langle f_W(X, k; t) \rangle_N \\ &\times \left[\cos(2pX/\hbar) - e^{-\epsilon X^2} \right] e^{-p^2/\epsilon \hbar^2}. \end{aligned} \quad (11)$$

A spatially modulated noise source, $g(X) = \alpha \sin(\beta X/\hbar)$, leads to

$$\frac{\partial}{\partial t} \langle f_W(X, k; t) \rangle_N = -L_{S_{y_0}} \langle f_W(X, k; t) \rangle_N$$

$$-\frac{B\Omega^2}{\pi\hbar^2} \cos^2(jX\hbar) [\langle f_W(X, k; t) \rangle_N - \frac{1}{2} \langle f_W(X, k - j; t) \rangle_N - \frac{1}{2} \langle f_W(X, k + j; t) \rangle_N] \quad (12)$$

It is clear that these equations are very different from the corresponding classical Fokker-Planck equations.

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