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NONLINEAR VON NEUMANN EQUATIONS FOR QUANTUM DISSIPATIVE SYSTEMS

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Abstract

For pure states nonlinear Schrödinger equations, the so-called Schrödinger-Langevin equations are well-known to model quantum dissipative systems of the Langevin type. For mixtures it is shown that these wave equations do not extend to master equations, but to corresponding non-linear von Neumann equations. Solutions for the damped harmonic oscillator are discussed.

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1. Pure States

The dynamics of quantum dissipative systems, describing a genuinely irreversible process can be formulated in the framework of non-Hamiltonian quantum statistics by means of a so-called quantum dynamical, ultraweakly continuous, completely positive semigroup which introduces a preferred direction in time. Let $\rho \in T_s(H)_1^+$ be a self-adjoint, positive trace class operator of trace equal to one on a separable, complex Hilbert space H. Then the density matrix at time t, ρ_t is given by the action of a time evolution contraction semigroup $\rho_t = \sigma_t \rho$. A quantum Langevin system is a particular model for a quantum dissipative system, defined by the equation of motion for the components of the position operator Q_k:

$$\frac{d^2}{dt^2} \mathrm{Tr}(\rho_t Q_k) + \gamma \frac{d}{dt} \mathrm{Tr}(\rho_t Q_k) = \mathrm{Tr}(\rho_t \frac{F_k}{m}) \quad (k = 1,\dots,d), \tag{1}$$

where F_k is a component of an external force. If $\rho_t = P_{\psi(t)}$ is a projector on a wave function $\psi(t) \in H$, then the following result holds for the existence of a Hamiltonian description of quantum Langevin systems [1]: For an irreducible representation of the CCR there do not exist an Hermitean, densely defined Hamiltonian which is the generator of an operator Langevin equation of motion corresponding to (1). Two possibilities have been explored to escape the conclusion of this theorem: First one can give up irreducibility by introducing a fluctuation force $F_s(t)$ in the operator Langevin equation of motion and use the stochastic Hamilton operator [2,3]

$$H = \sum_{i=1}^{d} \frac{1}{2m_i} \Delta_i e^{-\gamma t} + (V(x_1 \dots x_d) - \sum x_i F_{s,i}) e^{\gamma t} . \tag{2}$$

It is essential, in order not to violate the CCR, to interpret the wave function as a stochastic process. The random force is depending on variables characterizing the heat bath. Secondly one may introduce non-linear Hamiltonians for which adjoint operators cannot be defined, which amounts to giving up Hermiticity. In the sequel we shall be concerned with the latter case only. Essentially two types of nonlinear Schrödinger equations describing quantum Langevin systems are well-known. Kostin [4] introduced the so-called Schrödinger-Langevin equation of first type (SLE(I)) for $\psi \in \mathcal{D}(H) \cap \mathcal{D}(V_L) \subset L_2(\mathbb{R}^d, \mathbb{C}, d^dx)$

$$i \hbar \frac{\partial}{\partial t} \psi = H\psi + V_L(\psi)\, \psi \qquad (3)$$

with the Langevin potential

$$V_L(\psi) = \frac{\hbar\gamma}{2i} \left\{ \ln \frac{\psi}{\psi^*} - \int_{\mathbb{R}^d} \frac{|\psi|^2}{||\psi||_2^2} \ln \frac{\psi}{\psi^*}\, d^dx \right\} . \qquad (4)$$

V_L is a proper function of the complex plane with the following properties:

(a) $V_L(\psi) \in \mathbb{R}\,, \quad \forall\, \psi \in \mathcal{D}(V_L)$

which implies conservation of probability,

(b) $V_L(\omega\psi) = V_L(\psi)\,, \quad \forall\, \omega \in \mathbb{C}$

which implies normalizability of the wave function.

A second nonlinear wave equation used may be called the Schrödinger-Langevin equation of second type (SLE(II)):

$$i \hbar \frac{\partial}{\partial t} \psi = H\psi + W_L(\psi)\, \psi \quad , \tag{5}$$

$$W_L(\psi) = \gamma \sum_{k=1}^{d} (Q_k - \langle Q_k \rangle_\psi) \langle P_k \rangle_\psi \quad . \tag{6}$$

For A: $\mathcal{D} \subset L_2 \to L_2$ and $\psi \in \mathcal{D}$ we define

$$\langle A \rangle_\psi := \frac{(\psi, A\psi)}{||\psi||_2^2} \quad . \tag{7}$$

This equation has been introduced and generalized by several authors independently [5-8]. W_L shares the properties (a) and (b). Both equations are intimately related [1]. In case of the harmonic oscillator the solutions for the SLE(I) and SLE(II) are identical [9,1]. Confining ourselves to one dimension, these solutions read

$$\psi_n(z)(x,t) = e^{if(t)}\, e^{\frac{i}{\hbar} p_{cl} x}\, \phi_n(x - x_{cl}, t) \quad , \tag{8}$$

with $z = \sqrt{\frac{m\omega}{\hbar}}\, x_{cl} + i \frac{p_{cl}}{\sqrt{m\omega\hbar}}$. Hereby is f a differentiable real function of the time only, $n \in \mathbb{N}$, $p_{cl}(t) = m \frac{d}{dt} x_{cl}(t)$ and $x_{cl}(t)$ is a solution of the classical equation of motion of the damped harmonic oscillator. $\phi_n(y,t)$ are the stationary states of the undamped harmonic oscillator. They are also solutions of the damped problem (for $p_{cl} = x_{cl} = 0$).

2. Mixtures

For mixtures we are confronted with the following equation. Let H be a self-adjoint, in $L_2(\mathbb{R}^d)$ densely defined operator and $t \to \rho_t \in T_s(L_2)^+_1$ a strongly differentiable orbit and W an arbitrary (sufficiently smooth) function on $T_s(L_2)^+_1$. We call

$$\frac{\partial}{\partial t} \rho_t = - \frac{i}{\hbar} [H,\rho_t] + W(\rho_t) \tag{9}$$

a dissipative von Neumann equation (of Langevin type), corresponding to a dissipative Schrödinger equation (DSE) if

(A) $Tr(W(\rho)) = 0$.

(B) Let A_{xy} denote the kernel of the operator A with respect to the positions x and y, then $W(\rho)_{xy} = W(\rho)^{*}_{yx}$.

(C) $Tr(W(\rho)Q_k) = 0$, $(k = 1,\dots,d)$.

(D) $Tr(W(\rho)P_k) = -\gamma\, Tr(\rho P_k)$, $(k = 1,\dots,d)$.

(E) R is a solution of (9) and a projector if and only if R is a projector on a solution of the DSE.

(F) The time evolution induced by (9) maps the positive cone $T_s(L_2)^+$ into itself.

(G) (9) has at least one solution which is not a projector on a vector $\phi \in L_2$.

If $W = 0$, then $\gamma = 0$, and (9) is the usual von Neumann equation (corresponding to a non-dissipative, ordinary Schrödinger equation). If W is an affine function on $T_s(L_2)^+_1$, then (9) is called a master equation (or quantum mechanical Fokker-Planck equation [10]). Master equations, respectively the time evolution semigroups they describe are well founded by exactly solvable, rigorous microscopic models of open systems either in the weak coupling limit [11-14] or in the singular coupling limit [15,16]. Master equations show the important feature of preserving the convexity of the set of states.

No master equations however can correspond to the SLE(I) or SLE(II). It suffices to give a counterexample for the harmonic oscillator in one dimension. From quantum mechanics of the harmonic oscillator we know

$$e^{-\frac{1}{2}} \sum_n \left(\frac{1}{2}\right)^n \frac{1}{n!} \phi_n \otimes \phi_n^* = \int d^2z \, \frac{1}{2\pi} \, \delta(|z| - 1) \, \psi_o(z) \otimes \psi_o^*(z) \qquad (10)$$

with $d^2z = d \operatorname{Re} z \, d \operatorname{Im} z$ and $\psi_o(z)$ taken from (8).

First argument: Let $z_o = z(t = 0)$ then

$$\rho_1 = \int d^2z_o \, \frac{1}{2\pi} \, \delta(|z_o| - 1) \, \psi_o(z_o,t) \otimes \psi_o(z_o,t)^* \qquad (11)$$

and

$$\rho_2 = e^{-\frac{1}{2}} \sum_n \left(\frac{1}{2}\right)^n \frac{1}{n!} \phi_n \otimes \phi_n^* \qquad (12)$$

are two solutions of the master equation corresponding to the SLE(I) or SLE(II), which is supposed to exist. The initial conditions at $t = 0$ are

$$\rho_1(0) = \rho_2(0) = \rho_2(t) = \rho_2 \qquad (13)$$

but

$$\operatorname*{s-lim}_{t\to\infty} \rho_1(t) = \phi_o \otimes \phi_o^* \neq \rho_2 \qquad (14)$$

which contradicts the existence of unique solutions for master equations.

<u>Second argument</u>. We suppose there exists a master equation (9), i.e. W is affine. This equation corresponds to the SLE(I) or SLE(II):

$$W(\psi_n \otimes \psi_n^{*}) = -\frac{i}{\hbar}[Q,\gamma p_{cl}\ \psi_n \otimes \psi_n^{*}] \quad , \tag{15}$$

in particular

$$W(\phi_n \otimes \phi_n^{*}) = 0 \ . \tag{16}$$

From (10) we conclude

$$0 = \int d^2z\ \frac{1}{2\pi}\delta(|z| - 1)\ [Q,\gamma p_{cl}(z)\ \psi_o(z) \otimes \psi_o(z)] \quad , \tag{17}$$

which is easily checked to be false in contradiction to our supposition. With [17] and [10] we therefore conclude that the time evolution semigroup induced by the SLE(I) or SLE(II) cannot be extended to a norm or strongly continuous quantum dynamical semigroup on a von Neumann algebra.

Von Neumann equations corresponding to the SLE's are necessarily nonlinear. Therefore there arises a difficulty of interpretation: A density operator describes either an ensemble of subsystems in pure states or a single system in a mixed state. The non-affine evolution equation may be applied only in the second case. In the first case it is possible to observe any single subsystem of the ensemble separately: Since the subsystem is in a pure state, it evolves according to the SLE: $\rho_i(0) \to \rho_i(t)$ (i is the index for the subsystem, ρ_i its density operator which is a projection). If the density operator for the ensemble is

$\rho(0) = \frac{1}{N} \sum_{i=1}^{N} \rho_i(0)$ it is given at time t by $\rho(t) = \frac{1}{N} \sum_{i=1}^{N} \rho_i(t)$.

By inspection of the postulates (A) - (E) we found the following von Neumann-Langevin equation (vNLE(I)) corresponding to the SLE(I):

$$W(\rho) = V_L(\rho) = -\frac{1}{2}\gamma(\sqrt{\rho}\, V(\rho) + V(\rho)\sqrt{\rho}) \,, \tag{18}$$

$$V(\rho)_{xy} = (\sqrt{\rho})_{xy} \ln \frac{(\sqrt{\rho})_{xy}}{(\sqrt{\rho})_{yx}} \,. \tag{19}$$

As for the pure states the nonlinearity depends considerably on the representation chosen. A von Neumann-Langevin equation (vNLE(II)) corresponding to the SLE(II) is given by

$$W(\rho) = W_L(\rho) = -\frac{i}{\hbar}\gamma\,[Q,\rho]\,\mathrm{Tr}(\rho P) \,. \tag{20}$$

We emphasize that the shape of the generator W is not uniquely determined by the postulates (A) - (E). It is easily possible to give alternative formulas, e.g. for a vNLE(I). We chose the above forms because they are the most natural generalizations of the SLE's for mixtures and they show reasonable solutions.

Postulate (G) is verified for (18,19) and (20) by the following solutions for a one-dimensional harmonic oscillator, which are identical for both, the vNLE(I) and the vNLE(II): Let $\lambda_n \geq 0$, $\frac{\partial}{\partial t}\lambda_n = 0$ and $\sum_n \lambda_n = 1$, then

$$\rho_3 = \sum_n \lambda_n \psi_n \otimes \psi_n^* \tag{21}$$

and in particular (for $x_{cl} = p_{cl} = 0$)

$$\omega_4 = \sum_n \lambda_n \phi_n \otimes \phi_n^*$$

are solutions of the vNLE's. The proof is obtained by inserting (21) in (9) using (18,19) or (20) respectively.

A general proof that the positivity requirement (F) is satisfied by (18,19, or (20) remains an open problem.

Finally we remark that (21) is a solution of the vNLE(I) for which no entropy production arises. The vNLE(II) do not exhibit entropy production at all.

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