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Diffusive behaviour of solitons described by time-convolutionless generalized master equations

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Abstract. The time-convolutionless generalized master equation (GME) approach is implemented to analyse the dynamical behaviour of a new model for quantum dissipation that involves solitons as Brownian particles. The time evolution of the centre of the soliton and of the Wigner quasi-probability function is obtained as a function of the corresponding transport coefficients.

1. Introduction

Recently, Castro Neto and Caldeira [1] have presented a new model for quantum dissipation to describe the irreversible evolution of solitons in quantum field theory. Using the collective coordinate method [2] they have constructed an effective Hamiltonian for the soliton coupled to the residual excitations originated by the presence of the collective motion. By means of the functional integral formalism they showed that the soliton behaviour at low energies is like quantum Brownian behaviour due to the scattering of these renormalized excitations. This model exhibits very new features compared with those obtained in the standard quantum dissipative models like the damped oscillator [3] or spin relaxation [4], because in the present case the system and the reservoir are composed of the same constituents. In particular, this formulation has been shown to be useful in analysing a large class of physical systems like polarons [5], Bloch walls [6], and for those problems that involve solitons as solutions of the corresponding semi-classical equations of motion.

On the other hand, the time-convolutionless projection operator method [7] has proved to be a valuable tool for analysing the non-Markovian relaxation of an open quantum system described by a Hamiltonian of the system-plus-reservoir type. One of its many advantages is that very general conclusions about the behaviour of the system can be derived without reference to an explicit model for the thermal reservoir [8].

The purpose of this article is to examine the applicability of this formalism for the above stated model for solitons. In section 2 the time-convolutionless GME method is briefly reviewed and some necessary calculations are derived. The model is introduced in section 3 and the generalized master equation is constructed. The damped evolution of the soliton is analysed by means of the evolution of averages observables and the Wigner function. Finally, a specific model reservoir is examined. A summary of the results is given in section 4.

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2. The time-convolutionless GME

The dynamical behaviour of a system $\mathcal{S}$ which is coupled to a reservoir $\mathcal{R}$ can be computed from the knowledge of the reduced density operator

$$\sigma(t) = \mathrm{Tr}_{\mathrm{R}}\, \rho(t) \tag{2.1}$$

where Tr_{R} indicates tracing in the Hilbert space with respect to the quantum numbers of the reservoir $\mathcal{R}$ and $\rho(t)$ is the full $(\mathcal{S}+\mathcal{R})$ density operator that satisfies the Liouville equation

$$\frac{\partial}{\partial t}\rho(t) = \frac{\imath}{\hbar}\,[H, \rho(t)] \tag{2.2}$$

H being the total Hamiltonian of the composite system. In what follows, we will assume that this Hamiltonian takes the system-plus-reservoir form

$$H = H_{\mathrm{S}} + H_{\mathrm{R}} + \alpha H_{\mathrm{SR}} \tag{2.3}$$

where α scales the interaction strength for the combined system, and that the interaction term can be written in general form as

$$H_{\mathrm{SR}} = -SB \tag{2.4}$$

where S and B are hermitic operators on the Hilbert spaces of $\mathcal{S}$ and $\mathcal{R}$, respectively. As usual, the B operator contains infinite summations over all particles in the environment in order to obtain an irreversible behaviour of the system $\mathcal{S}$.

The time-convolutionless GME approach enables us to analyse the non-Markovian behaviour of the open quantum system described by (2.3). This method leads to a linear differential equation for the evolution of the reduced density matrix, which can be written [4] as

$$\frac{\partial}{\partial t}\sigma(t) + \frac{\imath}{\hbar}\,[H_{\mathrm{S}}, \sigma(t)] = \Lambda(t)\sigma(t) + J(t) \tag{2.5}$$

where $\Lambda(t)$ is the time-dependent collisional superoperator and the inhomogeneous term $J(t)$ is an operator which describes the evolution of the initial correlations. Although this term can be relevant in the short-time evolution, for our purposes it is sufficient to assume the uncorrelated initial condition

$$\rho(0) = \sigma(0)\rho_{\mathrm{R}}^{\mathrm{eq}} \tag{2.6}$$

being

$$\rho_{\mathrm{R}}^{\mathrm{eq}} = \mathrm{e}^{-\beta H_{\mathrm{R}}} / \,\mathrm{Tr}_{\mathrm{R}}\{\mathrm{e}^{-\beta H_{\mathrm{R}}}\} \tag{2.7}$$

the equilibrium reservoir density matrix at inverse temperature $\beta = 1/kT$. In this situation, one can verify that $J(t) = 0$ [4].

An expansion of the time-dependent rate coefficient $\Lambda(t)$ appearing in the GME (2.5) in powers of α can be obtained [7], being of the form

$$\Lambda(t) = \sum_n \alpha^n \Lambda_n(t)\,. \tag{2.8}$$

When the mean value of an odd number of reservoir operators B vanishes, the Λ_n terms can be simplified considerably. In particular, only even terms in the expansion survive. This is the usual assumption that has been considered in many applications in which H_{SR} is linear in the reservoir coordinates and/or the reservoir is purely harmonic. However, these conditions are not satisfied by the Hamiltonian that will be analysed, so the odd terms must be considered. After some algebra, the first two terms of the expansion (2.8) read

$$\Lambda_1(t)\sigma(t) = \frac{\imath}{\hbar}\,[S, \sigma(t)]\,\langle B(t)\rangle_{\mathrm{R}} \tag{2.9a}$$

$$\Lambda_2(t)\sigma(t) = -\frac{1}{\hbar^2}\int_0^t \mathrm{d}\tau\ \{[S, S(-\tau)\sigma(t)]\,\langle B(\tau)B\rangle_{\mathrm{R}} - [S, \sigma(t)S(-\tau)]\,\langle B(-\tau)B\rangle_{\mathrm{R}} - [S, [S(-\tau), \sigma(t)]]\,\langle B(t)\rangle_{\mathrm{R}}^2\} \tag{2.9b}$$

where

$$\langle B(t)\rangle_{\mathrm{R}} = \mathrm{Tr}_{\mathrm{R}}\{B(t)\rho_{\mathrm{R}}^{\mathrm{eq}}\} = \langle B\rangle_{\mathrm{R}} \tag{2.10}$$

is time independent, and

$$\langle B(t)B(\tau)\rangle_{\mathrm{R}} = \mathrm{Tr}_{\mathrm{R}}\{B(t)B(\tau)\rho_{\mathrm{R}}^{\mathrm{eq}}\} \tag{2.11}$$

is the correlation function of the reservoir operators [9] that satisfies

$$\langle B(t)B(\tau)\rangle_{\mathrm{R}} = \langle B(t-\tau)B\rangle_{\mathrm{R}} = \langle B(\tau-t)B\rangle_{\mathrm{R}}^* \ . \tag{2.12}$$

In these equations $S(t)$ ($B(t)$) must be computed in the non-interacting scheme for the system (reservoir).

Finally, up to second order (i.e. the Born approximation) the time-convolutionless generalized master equation (2.5) can be written as

$$\frac{\partial}{\partial t}\sigma(t) + \frac{\imath}{\hbar}\left[H_{\mathrm{S}} - \alpha S\,\langle B\rangle_{\mathrm{R}}\,, \sigma(t)\right] = -\frac{\alpha^2}{\hbar^2}\int_0^t \mathrm{d}\tau\ \ [S, [S(-\tau), \sigma(t)]]\,\{\Phi(\tau) - \langle B\rangle_{\mathrm{R}}^2\} - \imath\frac{\alpha^2}{\hbar^2}\int_0^t \mathrm{d}\tau\ \left[S, [S(-\tau), \sigma(t)]_+\right]\Psi(\tau) \tag{2.13}$$

where the symbols $[\ldots,\ldots]$ and $[\ldots,\ldots]_+$ respectively denote the commutator and anticommutator, while $\Phi(t)$ and $\Psi(t)$ are respectively the real and imaginary part of the correlation function, i.e.

$$\langle B(t)B\rangle_{\mathrm{R}} = \Phi(t) + \mathrm{i}\Psi(t)\,. \tag{2.14}$$

3. Evolution of a damped soliton

The irreversible dynamics of solitons at low energies can be described by an effective Hamiltonian of the form[1, 5]

$$H_{\mathrm{eff}} = \frac{1}{2M}\,[P-B]^2 + H_{\mathrm{R}}^{(0)} \tag{3.1}$$

where P is the momentum canonically conjugated to the coordinate Q that describes the centre of the soliton, $H_{\mathrm{R}}^{(0)}$ is a reservoir Hamiltonian of non-interacting particles and B is an infinite sum of reservoir operators.

To apply the results of the previous section one must set $S = P/M$ in (2.4) and

$$H_{\mathrm{S}} = \frac{P^2}{2M} \tag{3.2a}$$

$$H_{\mathrm{R}} = H_{\mathrm{R}}^{(0)} + B^2/2M\,. \tag{3.2b}$$

Then the corresponding GME can be derived substituting $S(t) = P(t)/M = P/M$ in (2.13), which becomes

$$\frac{\partial}{\partial t}\sigma(t) + \frac{\imath}{\hbar}\left[\frac{P^2}{2M} - \frac{P}{M}\langle B\rangle, \sigma(t)\right]$$

$$= -\frac{1}{(M\hbar)^2}[P,[P,\sigma(t)]]\int_0^t \mathrm{d}\tau\ \left(\Phi(\tau) - \langle B\rangle_{\mathrm{R}}^2\right)$$

$$-\frac{\imath}{(M\hbar)^2}\left[P,[P,\sigma(t)]_+\right]\int_0^t \mathrm{d}\tau\ \Psi(\tau)\,. \tag{3.3}$$

This equation can be rewritten as

$$\frac{\partial}{\partial t}\sigma(t) + \frac{\imath}{\hbar}[H_{\mathrm{ren}}, \sigma(t)] = -\frac{C(t)}{\hbar^2}[P,[P,\sigma(t)]] \tag{3.4}$$

where

$$H_{\mathrm{ren}} = \frac{P^2}{2M}f(t) - \frac{P}{M}\langle B\rangle_{\mathrm{R}} \tag{3.5}$$

plays the role of a renormalized Hamiltonian [9], $f(t)$ being given by

$$f(t) = 1 + \frac{2}{M\hbar}\int_0^t \mathrm{d}\tau\ \Psi(\tau) \tag{3.6}$$

while

$$C(t) = \frac{1}{M^2}\int_0^t \mathrm{d}\tau\ \left(\Phi(\tau) - \langle B\rangle_{\mathrm{R}}^2\right) \tag{3.7}$$

is the time-dependent diffusion coefficient, as we shall see below.

Note that the non-Markovian behaviour of the GME (3.4) is only present in the temporal dependence of its coefficients and this characteristic is lost if one adopts the more traditional convolution master equation approach. On the other hand, if one considers a correlated initial density instead of (2.6) these coefficients remain unchanged.

3.1. Mean values

Using the fact that $\langle A\rangle_t = \mathrm{Tr}_{\mathrm{S}}\{A\sigma(t)\}$ for an operator A belonging to the soliton space, from (3.4) we obtain

$$\langle\dot{Q}\rangle = f(t)\frac{\langle P\rangle}{M} - \frac{\langle B\rangle_{\mathrm{R}}}{M} \tag{3.8a}$$

$$\langle\dot{P}\rangle = 0 \tag{3.8b}$$

showing the property that P is a constant of motion and cannot be the soliton momentum [1]. This can be easily verified for the form of the total Hamiltonian (3.1).

It is worth noting that from equations (3.8) one can write

$$M\langle\ddot{Q}\rangle - M\frac{\dot{f}(t)}{f(t)}\langle\dot{Q}\rangle = \frac{\dot{f}(t)}{f(t)}\langle B\rangle_{\mathrm{R}} \tag{3.9}$$

that describes a damped evolution of the centre of the soliton. The corresponding time-dependent friction coefficient reads

$$\nu(t) = -M\frac{\dot{f}(t)}{f(t)} = -M\frac{\partial}{\partial t}\ln f(t) = -\frac{2}{\hbar}\Psi(t) \tag{3.10}$$

where the last equality holds in the Born approximation.

Therefore, the friction coefficient has the same temporal behaviour of the imaginary part of the reservoir correlations and must decay to zero for times greater than the characteristic time τ_R of these correlations. So, for times $t \gg \tau_R$ we obtain $\nu(t) \to 0$, and the mean value of the centre of the soliton evolves in time as a free particle.

In particular, the solution of equations (3.8) is given by

$$\langle Q\rangle_t = \langle Q\rangle_0 + \frac{\langle P\rangle_0}{M}\left(t + \frac{2}{M\hbar}\int_0^t \mathrm{d}\tau \int_0^\tau \mathrm{d}\tau'\ \Psi(\tau')\right) - \frac{\langle B\rangle_R}{M}t \qquad (3.11)$$

It must be stressed that the above results are very different from those obtained in the usual Brownian motion, which can be derived setting $S = Q$ in (2.4). In the latter case the friction coefficient tends to a finite value, so the behaviour is always damped.

3.2. Evolution of the Wigner quasi-probability function

Another way to extract useful information about the GME (3.4) is to give its semi-classical counterpart by means of the Wigner representation [10]

$$\sigma_W(Q, P, t) = \int \mathrm{d}v\ \mathrm{e}^{\mathrm{i}Pv/\hbar}\left\langle Q - \frac{v}{2}|\sigma\,(t)|Q + \frac{v}{2}\right\rangle . \qquad (3.12)$$

If one take into account the same prescriptions as in [11], some straightforward algebra leads to the semi-classical equation of motion for the Wigner quasi-probability function, which is given by

$$\frac{\partial}{\partial t}\sigma_W(Q, t) = \left\{-D(t)\frac{\partial}{\partial Q} + C(t)\frac{\partial^2}{\partial Q^2}\right\}\sigma_W(Q, t) \qquad (3.13)$$

where

$$D(t) = f(t)\frac{P}{M} - \frac{\langle B\rangle_R}{M} . \qquad (3.14)$$

Since P is a constant of motion, equation (3.13) is a generalized Fokker–Planck equation for one variable [12], being $D(t)$ the time-dependent drift coefficient while $C(t)$ is now easily identified as the time-dependent diffusion coefficient.

One must realize here that in the quantum case fluctuations and dissipation involve different temperature-dependent time scales [13], because the time behaviour of the real and imaginary part of the correlation function (2.11) strongly depends on the explicit form of the operator B. In what follows, τ_R is taken as the longer of these two time scales.

The Fokker–Planck equation (3.13) can be analytically solved making use of the Fourier transform

$$\tilde{\sigma}(k, t) = \int \mathrm{e}^{-\mathrm{i}kQ}\sigma_W(Q, t)\ \mathrm{d}Q \qquad (3.15)$$

from which

$$\frac{\partial}{\partial t}\tilde{\sigma}(k, t) = -\left(\mathrm{i}kD(t) + k^2C(t)\right)\tilde{\sigma}(k, t) . \qquad (3.16)$$

Using the initial condition $\sigma_W(Q, 0) = \delta(Q - Q_0)$, then $\tilde{\sigma}(k, 0) = \mathrm{e}^{-\mathrm{i}kQ_0}$ and the solution of (3.13) is

$$\sigma_W(Q, t) = \frac{1}{\sqrt{4\pi c(t)}}\exp\left\{-\frac{(Q - Q_0 - d(t))^2}{4c(t)}\right\} \qquad (3.17)$$

where

$$d(t) = \int_0^t \mathrm{d}\tau\ D(\tau) = \frac{P}{M}\left(t + \frac{2}{M\hbar}\int_0^t \mathrm{d}\tau \int_0^\tau \mathrm{d}\tau'\ \Psi(\tau')\right) - \frac{\langle B\rangle_\mathrm{R}}{M}t \tag{3.18a}$$

$$c(t) = \int_0^t \mathrm{d}\tau\ C(\tau) = \frac{1}{M^2}\int_0^t \mathrm{d}\tau \int_0^\tau \mathrm{d}\tau'\ \left(\Phi(\tau') - \langle B\rangle_\mathrm{R}^2\right)\ . \tag{3.18b}$$

Therefore, $\sigma_\mathrm{W}(Q, t)$ is a Gaussian distribution whose centre moves as $Q_0 + d(t)$ while its width grows as $\sqrt{c(t)}$. Notice that if the interaction is turned off $f(t) = 1$. Then $\sigma_W(Q, t) = \delta(Q - Q_0 - (P/M)t)$ and, as we would expect the soliton moves as a free particle with velocity P/M. After the reservoir correlations have decayed ($t > \tau_\mathrm{R}$) the centre of the soliton acquires a diffusive behaviour with constant drift and diffusion coefficients.

3.3. *Explicit example*

In the foregoing sections we have not made any assumption about the form of the reservoir operator B. From now on we shall study the situation described in [1], in which the reservoir is given by

$$H_\mathrm{R}^{(0)} = \sum_n \hbar\Omega_n b_n^\dagger b_n \tag{3.19a}$$

$$B = \sum_{nm} \hbar g_{nm} b_m^\dagger b_n \tag{3.19b}$$

where $b_n^\dagger$ and b_n are the usual creation and annihilation boson operators, while g_{nm} are coupling constants obeying $g_{nm} = -g_{mn}$.

In order to calculate the mean values (2.10) and (2.11), the propagator

$$\left\langle\alpha\right|\exp\!\left(-\imath t(H_\mathrm{R}^{(0)} + B^2)/\hbar\right)\left|\beta\right\rangle$$

must be evaluated. However, the term containing B^2 in the exponential makes it very difficult and an expansion can be implemented. To first order, the exponential involved is evaluated taking $H_\mathrm{R} \approx H_\mathrm{R}^{(0)}$, giving

$$\langle B\rangle_\mathrm{R} = 0 \tag{3.20}$$

and, using the Wick theorem, one obtains

$$\langle B(t)B\rangle_\mathrm{R} = -\sum_{nm} \hbar^2 g_{nm}^2 \mathrm{e}^{\imath(\Omega_n - \Omega_m)t}(\bar{n}_m + 1)\bar{n}_n \tag{3.21}$$

where

$$\bar{n}_n = \frac{1}{\mathrm{e}^{\beta\hbar\Omega_n} - 1} \tag{3.22}$$

is the average number of elementary excitations of given type n. In this case, the real and imaginary part of the correlation function can be written as

$$\Phi(\tau) = -\sum_{nm} \hbar^2 g_{nm}^2 (\bar{n}_m + 1)\bar{n}_n \cos(\Omega_n - \Omega_m)t \tag{3.23a}$$

$$\Psi(\tau) = -\sum_{nm} \hbar^2 g_{nm}^2 (\bar{n}_m + 1)\bar{n}_n \sin(\Omega_n - \Omega_m)t\ . \tag{3.23b}$$

At zero temperature $\bar{n}_n = 0$ and then the correlation function (3.23) vanished, so $f(t) = 1$ and $C(t) = 0$. Therefore, in this situation one can conclude as in [1] that the soliton moves freely. This fact can be easily understood noting that at zero temperature the coupling Hamiltonian terms $b_m^\dagger b_n$ are only acting over the reservoir ground state. At finite temperature the reservoir excitations are activated and can scatter off the soliton, which acquires a diffusive behaviour.

Introducing the scattering function [1]

$$S(\omega, \omega') = \sum_{n,m} \hbar^2 g_{nm}^2 \delta(\omega - \Omega_n)\delta(\omega' - \Omega_m) \tag{3.24}$$

one finds that the transport coefficients can be written as

$$\nu(t) = \frac{2}{\hbar} \int \mathrm{d}\omega \int \mathrm{d}\omega' \; S(\omega, \omega')\bar{n}(\omega)(\bar{n}(\omega') + 1) \sin(\omega - \omega')t \tag{3.25a}$$

$$C(t) = -\frac{1}{M^2} \int \mathrm{d}\omega \int \mathrm{d}\omega' \; S(\omega, \omega')\bar{n}(\omega)(\bar{n}(\omega') + 1)) \frac{\sin(\omega - \omega')t}{(\omega - \omega')} \tag{3.25b}$$

which are in agreement with expressions obtained in [14] using the functional integral formalism.

At this point I wish to stress that the effective Hamiltonian (3.1) together with (3.19) have recently been used to analyse the dissipative motion of different kinds of systems. This model allows one to treat the strong-coupling limit of an electron interacting with a lattice [5], reducing this problem to the case of a polaron (the soliton) in the presence of renormalized phonons. Another example can be found in magnetic systems, when one considers a ferromagnetic XYZ model [6]. In this case soliton-like solutions of the nonlinear equation which controls the spin dynamics can be obtained, the so-called Bloch walls, which interact with a magnon reservoir. For both examples, the transport coefficients will have the functional form (3.25). However, the characteristic times will strongly depend on the explicit form of the scattering function (3.24) via the coupling constants g_{nm} [15], which are obtained when one applies the collective coordinate method to the specific problem.

4. Summary

In this work, we implement the time-convolutionless GME method to analyse the irreversible behaviour of solitons. A remarkable feature of this method is that it enables us to obtain some general conclusions regarding the behaviour of the soliton without making any assumption about the specific form of the reservoir. In this sense, the evolution of the mean values and the Wigner quasi-probability function can easily be obtained and the time-dependent transport coefficients can be identified. In particular, one can observe that initially the mean value of the coordinate that represents the centre of the soliton describes a damped evolution with a friction coefficient that decays to zero for times greater than the characteristic time of the reservoir correlations. After the reservoir correlations have decayed, the soliton acquires a net diffusive behaviour that can be described by a Fokker–Planck equation.

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