Universidad Nacional de Colombia

Master of Science in Physics Thesis

Quantum Trajectories in non-Markovian system via the reaction coordinate mapping.

Autor:
Luis Eduardo Herrera Rodríguez
C.c: 1049650402
Email: leherrerar@unal.edu.co

Director:
Carlos Leonardo Viviescas
Physics PhD.

Facultad de Ciencia- Física

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Abstract.

1 Introduction

In the last two decades, experimental advances in quantum physics have made possible to prepare and manipulate quantum systems in large and complex ways. Nowadays, tens of ions can be trapped and transported at will in microtraps, quantum trajectories can be observed using superconducting qubits in microwave cavities, optical lattices are used to interfere clouds of cold bosons, and nanoparticles can be levitated and cooled to low temperatures[1, 2, 3, 4].

This make quantum information processing and quantum technologies one of the most promising applications of quantum theory, but one of the biggest challenges is to have detailed and specific control over each and all of the constituents of a quantum system. This difficulties arises form the fact that the system couples with his environment, which usually one only have partial control of it, changing the dynamics of the interest system, in result the dynamics is difficult to get due to the effect of the environment on the system. To overcome this problem and get the dynamics of the system, taking in account the irreversible and non-unitary processes (like dissipation, decoherence or measurement process), one have to employ a master equation description. The Limbland equation is the most general master equation for open quantum systems, but is restricted to the regime of weak coupling and Markovian environment.

Meantime, the macroscopic thermodynamics and classical statistical physics have move towards systems with smaller scales, aiming to construct a new thermodynamic framework that has in account the finite size effects, the non-equilibrium dynamics, the quantum properties and goes beyond the conventional regime of validity of macroscopic thermodynamics.

2 Dissipative systesm: Caldeira Legget Hamiltonian

full fish Here we talk about the Caldeira Legget Hamiltonian

3 The Reaction Coordinate map with classicl variables

Here we make the RC mapping for q and p

4 The spin Boson model with a two level system

we have the model

$$H = H_s + S\sum_k \left(h_k a_k + h_k^* a_k^\dagger\right) + \sum_k \omega_k a_k^\dagger a_k \tag{1}$$

Where H_s is the system which one is interested in his dynamics and is coupled to the bosonic bath, S denotes a dimensionless operator that acts only in the system ($S = S \otimes \mathbb{I}$), $a_k^\dagger(a_k)$ are the creation (annihilation) operator for the bosonic bath with modes frequencies ω_k, which are coupled linearly with the system with strength h_k, and fulfill the bosonic commutation relations $\left[a_k, a_{k'}^\dagger\right] = \delta_{k,k'}$.

Here talk about the spectral density.

$$\Gamma(\omega) = 2\pi \sum_k |h_k|^2 \, \delta(\omega - \omega_k) \tag{2}$$

5 Quantum dot coupled to 2 baths

6 The Reaction Coordinate map with bosonic creation and anhilation operators

We desire a map such that the new mapped Hamiltonian has the form:

$$H = H_s + \lambda S\left(b + b^\dagger\right) + \Omega b^\dagger b + (b + b^\dagger)\sum_{k\neq 1}\left(H_k b_k + H_k^* b_k^\dagger\right) + \sum_{k\neq 1}\Omega_k b_k^\dagger b_k \tag{3}$$

where the $b_k^\dagger(b_k)$ are the creation (annihilation) operator for the new bosonic bath with modes frequencies Ω_k, which are coupled linearly with the system with strength H_k, and fulfill the bosonic commutation relations $[b_k, b_{k'}^\dagger] = \delta_{k,k'}$. To achieve this purpose the map can be done by applying a Bogoliubov transformation, where the annihilation operators a_k are linearly transformed into new modes b_k:

$$a_k = u_{k1}b_1 + \sum_{q\neq 1} u_{kq}b_q + v_{k1}b_1^\dagger + \sum_{q\neq 1} v_{kq}b_q^\dagger, \tag{4}$$

The distinction is made with respect b_1 because this mode will be selected as the reaction coordinate ($b = b_1$). In order to preserve the bosonic commutations relation, the Bogoliubov transformation should be sympetic, i.e. the matirces $\mathbf{U}$ and $\mathbf{V}$ with complex coeffients $u_k q$ and $v_k q$ respectively obey $\mathbf{U}\mathbf{U}^\dagger - \mathbf{V}\mathbf{V}^\dagger = \mathbb{I}$ and $\mathbf{U}\mathbf{U}^T - \mathbf{V}\mathbf{U}^T = \mathbf{0}$. The construction of the sympletic tranformation can be donde with an orthogonal tranformation such the matrices elements are :

$$u_{kq} = \frac{1}{2}\left(\frac{\bar{a_k}}{\bar{b_q}} + \frac{\bar{b_k}}{\bar{a_q}}\right)\Lambda_{kq}, \qquad v_{kq} = \frac{1}{2}\left(\frac{\bar{a_k}}{\bar{b_q}} - \frac{\bar{b_k}}{\bar{a_q}}\right)\Lambda_{kq}, \tag{5}$$

where $\bar{a_k}$ and $\bar{b_k}$ are real valued and Λ_{kq} is a orthogonal matrix, imposing $\sum_q \Lambda_{kq}\Lambda_{kq'} = \delta_{k,k'}$.

For characterizin the new bath is need the new spectral density, following the convention we have:

$$\Gamma^{(1)}(\omega) = 2\pi\sum_k |H_k|^2\,\delta(\omega - \Omega_k). \tag{6}$$

For this bosonic map (phonon mapping) we can choose > 0, since we can introduce a phase in the b_k modes leading to a phase change in the H_k coefficient, in the same fashion we can define h_k to be real value coefficient. Then the mapping take the form:

$$u_{kq} = \frac{1}{2}\left(\sqrt{\frac{\omega_k}{\Omega_k}} + \sqrt{\frac{\Omega_k}{\omega_k}}\right)\Lambda_{kq}, \qquad v_{kq} = \frac{1}{2}\left(\sqrt{\frac{\omega_k}{\Omega_k}} - \sqrt{\frac{\Omega_k}{\omega_k}}\right)\Lambda_{kq}, \tag{7}$$

Then the last term of equation 1 in transformed as:

$$\sum_k \omega_k a_k^\dagger a_k =$$
$$\sum_k \omega_k \left[u_{k1} b^\dagger + \sum_{q\neq 1} u_{kq} b_q^\dagger + v_{k1} b + \sum_{q\neq 1} v_{kq} b_q \right] \left[u_{k1} b_1 + \sum_{q\neq 1} u_{kq} b_q + v_{k1} b_1^\dagger + \sum_{q\neq 1} v_{kq} b_q^\dagger \right] \quad (8)$$

We will separate the terms of 8 depending if they are related with the RC, and for the moment we will not take the sumatory over k. The terms related with the RC are:

$$\begin{aligned} u_{k1}u_{k1}b^\dagger b + \sum_{q\neq 1} u_{k1}u_{kq}b^\dagger b_q + u_{k1}v_{k1}b^\dagger b^\dagger + \sum_{q\neq 1} u_{k1}v_{kq}b^\dagger b_q^\dagger + \\ v_{k1}u_{k1}bb + \sum_{q\neq 1} v_{k1}u_{kq}bb_q + v_{k1}v_{k1}bb^\dagger + \sum_{q\neq 1} v_{k1}v_{kq}bb_q^\dagger + \\ \sum_{q\neq 1} u_{k1}u_{kq}b_q^\dagger b + \sum_{q\neq 1} v_{k1}u_{kq}b_q^\dagger b^\dagger + \sum_{q\neq 1} u_{k1}v_{kq}b_q b + \sum_{q\neq 1} v_{k1}v_{kq}b_q b^\dagger, \end{aligned} \quad (9)$$

and the terms without the RC:

$$\sum_{q,q'\neq 1} u_{kq}u_{kq'}b_{q'}^\dagger b_q + \sum_{q,q'\neq 1} u_{kq'}v_{kq}b_{q'}^\dagger b_q^\dagger + \sum_{q,q'\neq 1} v_{kq'}u_{kq}b_{q'}b_q + \sum_{q,q'\neq 1} v_{kq'}v_{kq}b_{q'}b_q^\dagger \quad (10)$$

Now we will work with the terms without the RC, usign the commutation relation for the new modes $[b_q, b_{q'}^\dagger] = \delta_{qq'}$ we have that equation 10 becomes :

$$\underbrace{\sum_{q,q'\neq 1} \left(u_{kq}u_{kq'} + v_{kq}v_{kq'}\right) b_{q'}^\dagger b_q}_{part\ 1} + \overbrace{\sum_{q,q'\neq 1} u_{kq'}v_{kq}\left(b_{q'}^\dagger b_q^\dagger + b_q b_{q'}\right)}^{part\ 2} + \underbrace{\sum_{q,q'\neq 1} v_{kq'}v_{kq}\delta_{qq'}}_{part\ 3} \quad (11)$$

Taking the sum over k we can impose that the new coordiantes(operators) will be in normal form for part 1:

$$\sum_k \omega_k \sum_{q,q'\neq 1} \left(u_{kq}u_{kq'} + v_{kq}v_{kq'}\right) b_{q'}^\dagger b_q = \sum_{q\neq 1} \Omega_q b_{q'}^\dagger b_q, \quad (12)$$

leading to the condition

$$\Omega_q \delta_{qq'} = \sum_k \omega_k \left(u_{kq}u_{kq'} + v_{kq}v_{kq'}\right) \quad (13)$$

whitch can be resume in:

$$\boxed{\Omega_q \Omega_{q'} \delta_{qq'} = \sum_k \omega_k^2 \Lambda_{kq} \Lambda_{kq'}} \quad (14)$$

Taking the sum over k for the second part and using the orthogonality condition $\sum_k \Lambda_{kq}\Lambda_{kq'} = \delta_{qq'}$, one get:

$$\sum_k \omega_k \sum_{q,q'\neq 1} u_{kq'} v_{kq} \left(b^\dagger_{q'} b^\dagger_q + b_q b_{q'} \right) = \sum_{q,q'\neq 1} \frac{1}{4} \frac{1}{\sqrt{\Omega_q \Omega_{q'}}} \left(\Omega_q - \Omega_{q'} \right) \sum_k \omega_k \Lambda_{kq} \Lambda_{kq'}, \tag{15}$$

changing the index $q \rightarrow q'$, is easy to see that this term is cero.

And the part 3 using $\sum_k \omega_k^2 \Lambda_{kq}^2 = \Omega_q^2$ and $\sum_k \Lambda_{kq}^2 = 1$:

$$\sum_k \omega_k \sum_{q,q'\neq 1} v_{kq'} v_{kq} \delta_{qq'} = \frac{1}{2} \sum_{q\neq 1} \left(\Omega_q - \sum_k \omega_k \Lambda_{kq}^2 \right) \tag{16}$$

7 The Reaction Coordinate map with fermionic creation and annihilation operators

8 Master Equation

9 Quantum Trajectories

10 Non-Markovian Dynamics

11 References

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